

Connecting via Winsock to STN

Welcome to STN International! Enter x:x

LOGINID:SSPTACXB1654

PASSWORD:

TERMINAL (ENTER 1, 2, 3, OR ?):2

* * * * * Welcome to STN International * * * * *

NEWS	1		Web Page for STN Seminar Schedule - N. America
NEWS	2	JUL 28	CA/Caplus patent coverage enhanced
NEWS	3	JUL 28	EPFULL enhanced with additional legal status information from the epoline Register
NEWS	4	JUL 28	IFICDB, IFIPAT, and IFIUDB reloaded with enhancements
NEWS	5	JUL 28	STN Viewer performance improved
NEWS	6	AUG 01	INPADOCDB and INPAFAMDB coverage enhanced
NEWS	7	AUG 13	CA/Caplus enhanced with printed Chemical Abstracts page images from 1967-1998
NEWS	8	AUG 15	CAOLD to be discontinued on December 31, 2008
NEWS	9	AUG 15	Caplus currency for Korean patents enhanced
NEWS	10	AUG 27	CAS definition of basic patents expanded to ensure comprehensive access to substance and sequence information
NEWS	11	SEP 18	Support for STN Express, Versions 6.01 and earlier, to be discontinued
NEWS	12	SEP 25	CA/Caplus current-awareness alert options enhanced to accommodate supplemental CAS indexing of exemplified prophetic substances
NEWS	13	SEP 26	WPIDS, WPINDEX, and WPIX coverage of Chinese and Korean patents enhanced
NEWS	14	SEP 29	IFICLS enhanced with new super search field
NEWS	15	SEP 29	EMBASE and EMBAL enhanced with new search and display fields
NEWS	16	SEP 30	CAS patent coverage enhanced to include exemplified prophetic substances identified in new Japanese-language patents
NEWS	17	OCT 07	EPFULL enhanced with full implementation of EPC2000
NEWS	18	OCT 07	Multiple databases enhanced for more flexible patent number searching
NEWS	19	OCT 22	Current-awareness alert (SDI) setup and editing enhanced
NEWS	20	OCT 22	WPIDS, WPINDEX, and WPIX enhanced with Canadian PCT Applications
NEWS	21	OCT 24	CHEMLIST enhanced with intermediate list of pre-registered REACH substances
NEWS EXPRESS	JUNE 27 08	CURRENT WINDOWS VERSION IS V8.3,	
		AND CURRENT DISCOVER FILE IS DATED 23 JUNE 2008.	
NEWS HOURS	STN Operating Hours Plus Help Desk Availability		
NEWS LOGIN	Welcome Banner and News Items		
NEWS IPC8	For general information regarding STN implementation of IPC 8		

Enter NEWS followed by the item number or name to see news on that specific topic.

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* * * * * STN Columbus * * * * *

FILE 'HOME' ENTERED AT 18:12:29 ON 11 NOV 2008

=> fil reg

COST IN U.S. DOLLARS

SINCE FILE

TOTAL

ENTRY

SESSION

FULL ESTIMATED COST

0.21

0.21

FILE 'REGISTRY' ENTERED AT 18:12:36 ON 11 NOV 2008

USE IS SUBJECT TO THE TERMS OF YOUR STN CUSTOMER AGREEMENT.

PLEASE SEE "HELP USAGETERMS" FOR DETAILS.

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Property values tagged with IC are from the ZIC/VINITI data file provided by InfoChem.

STRUCTURE FILE UPDATES: 10 NOV 2008 HIGHEST RN 1071907-21-5

DICTIONARY FILE UPDATES: 10 NOV 2008 HIGHEST RN 1071907-21-5

New CAS Information Use Policies, enter HELP USAGETERMS for details.

TSCA INFORMATION NOW CURRENT THROUGH July 5, 2008.

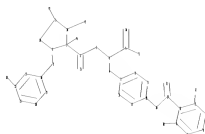
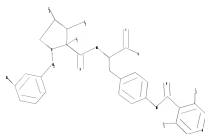
Please note that search-term pricing does apply when conducting SmartSELECT searches.

REGISTRY includes numerically searchable data for experimental and predicted properties as well as tags indicating availability of experimental property data in the original document. For information on property searching in REGISTRY, refer to:

<http://www.cas.org/support/stngen/stndoc/properties.html>

=>

Uploading C:\Program Files\Stnexp\Queries\10591820 formula I A is N.str



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chain nodes :
2  3  4  5  6  17  24  25  26  27  28  29  31  37  38  42  43  45
ring nodes :
1  7  8  9  10  11  12  13  14  15  16  18  19  20  21  22  23  30  32  33  34  35
36
chain bonds :
1-2  1-45  2-3  2-25  3-4  4-5  4-6  5-26  5-27  6-7  10-28  13-17  15-42  16-43
17-18  22-24  28-29  29-30  29-31  32-37  36-38
ring bonds :
1-13  1-16  7-8  7-12  8-9  9-10  10-11  11-12  13-14  14-15  15-16  18-19  18-23
19-20  20-21  21-22  22-23  30-32  30-36  32-33  33-34  34-35  35-36
exact/norm bonds :
1-13  1-16  1-45  2-3  2-25  3-4  5-26  5-27  10-28  13-14  13-17  14-15  15-16
15-42  16-43  28-29  29-31  32-37  36-38
exact bonds :
1-2  4-5  4-6  6-7  17-18  22-24  29-30
normalized bonds :
7-8  7-12  8-9  9-10  10-11  11-12  18-19  18-23  19-20  20-21  21-22  22-23  30-32
30-36  32-33  33-34  34-35  35-36

```

G1:X,MeO,EtO,n-PrO,i-PrO,CH₃,CH₂,CH,Et,n-Pr,i-Pr

G2:H,N

G3:H,CH3

Match level :

1:Atom 2:CLASS 3:CLASS 4:CLASS 5:CLASS 6:CLASS 7:Atom 8:Atom 9:Atom
10:Atom 11:Atom 12:Atom 13:Atom 14:Atom 15:Atom 16:Atom 17:CLASS 18:Atom
19:Atom 20:Atom 21:Atom 22:Atom 23:Atom 24:CLASS 25:CLASS 26:CLASS 27:CLASS
28:CLASS 29:CLASS 30:Atom 31:CLASS 32:Atom 33:Atom 34:Atom 35:Atom 36:Atom
37:CLASS 38:CLASS 42:CLASS 43:CLASS 45:CLASS

L1 STRUCTURE UPLOADED

=> d l1

L1 HAS NO ANSWERS

L1 STR

* STRUCTURE DIAGRAM TOO LARGE FOR DISPLAY - AVAILABLE VIA OFFLINE PRINT *

Structure attributes must be viewed using STN Express query preparation.

=> s l1 sam

SAMPLE SEARCH INITIATED 18:13:03 FILE 'REGISTRY'

SAMPLE SCREEN SEARCH COMPLETED - 11 TO ITERATE

100.0% PROCESSED 11 ITERATIONS 10 ANSWERS

SEARCH TIME: 00.00.01

FULL FILE PROJECTIONS: ONLINE **COMPLETE**

BATCH **COMPLETE**

PROJECTED ITERATIONS: 22 TO 418

PROJECTED ANSWERS: 11 TO 389

L2 10 SEA SSS SAM L1

=> s l1 full

FULL SEARCH INITIATED 18:13:10 FILE 'REGISTRY'

FULL SCREEN SEARCH COMPLETED - 127 TO ITERATE

100.0% PROCESSED 127 ITERATIONS 102 ANSWERS

SEARCH TIME: 00.00.01

L3 102 SEA SSS FUL L1

=> d scan

L3 102 ANSWERS REGISTRY COPYRIGHT 2008 ACS on STN

IN L-Phenylalanine, (4R)-1-[(3-cyanophenyl)sulfonyl]-4-(3-methyl-1-piperidinyl)-L-prolyl-4-[[[(3,5-dichloro-4-pyridinyl)carbonyl]amino]-ethyl ester, mono(trifluoroacetate) (9CI)

MF C35 H38 Cl2 N6 O6 S . C2 H F3 O2

CM 1

Absolute stereochemistry.



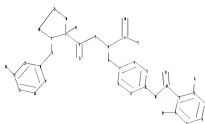
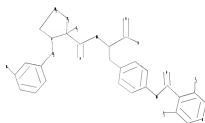
Please note that search-term pricing does apply when conducting SmartSELECT searches.

REGISTRY includes numerically searchable data for experimental and predicted properties as well as tags indicating availability of experimental property data in the original document. For information on property searching in REGISTRY, refer to:

<http://www.cas.org/support/stngen/stdoc/properties.html>

=>

Uploading C:\Program Files\Stnexp\Queries\10591820 not.str



```
chain nodes :
2  3  4  5  6  17  24  25  26  27  28  29  31  37  38  43
ring nodes :
1  7  8  9  10  11  12  13  14  15  16  18  19  20  21  22  23  30  32  33  34  35
36
chain bonds :
1-2  1-43  2-3  2-25  3-4  4-5  4-6  5-26  5-27  6-7  10-28  13-17  17-18  22-24
28-29  29-30  29-31  32-37  36-38
ring bonds :
1-13  1-16  7-8  7-12  8-9  9-10  10-11  11-12  13-14  14-15  15-16  18-19  18-23
19-20  20-21  21-22  22-23  30-32  30-36  32-33  33-34  34-35  35-36
exact/norm bonds :
1-13  1-16  1-43  2-3  2-25  3-4  5-26  5-27  10-28  13-14  13-17  14-15  15-16
28-29  29-31  32-37  36-38
exact bonds :
```

1-2 4-5 4-6 6-7 17-18 22-24 29-30
normalized bonds :
7-8 7-12 8-9 9-10 10-11 11-12 18-19 18-23 19-20 20-21 21-22 22-23 30-32
30-36 32-33 33-34 34-35 35-36

G1:X,MeO,EtO,n-PrO,i-PrO,CH3,CH2,CH,Et,n-Pr,i-Pr

G2:H,N

G3:H,CH3

Match level :

1:Atom 2:CLASS 3:CLASS 4:CLASS 5:CLASS 6:CLASS 7:Atom 8:Atom 9:Atom
10:Atom 11:Atom 12:Atom 13:Atom 14:Atom 15:Atom 16:Atom 17:CLASS 18:Atom
19:Atom 20:Atom 21:Atom 22:Atom 23:Atom 24:CLASS 25:CLASS 26:CLASS 27:CLASS
28:CLASS 29:CLASS 30:Atom 31:CLASS 32:Atom 33:Atom 34:Atom 35:Atom 36:Atom
37:CLASS 38:CLASS 43:CLASS

L4 STRUCTURE UPLOADED

=> s 14 sam subset=13

SAMPLE SUBSET SEARCH INITIATED 18:15:13 FILE 'REGISTRY'

SAMPLE SUBSET SCREEN SEARCH COMPLETED - 10 TO ITERATE

100.0% PROCESSED 10 ITERATIONS

0 ANSWERS

SEARCH TIME: 00.00.01

PROJECTIONS (WITHIN SPECIFIED SUBSET):

ONLINE

COMPLETE

PROJECTED ITERATIONS (WITHIN SPECIFIED SUBSET):

11 TO

389

PROJECTED ANSWERS (WITHIN SPECIFIED SUBSET):

0 TO

0

L5 0 SEA SUB=L3 SSS SAM L4

=> s 14 full subset=13

FULL SUBSET SEARCH INITIATED 18:15:21 FILE 'REGISTRY'

FULL SUBSET SCREEN SEARCH COMPLETED - 102 TO ITERATE

100.0% PROCESSED 102 ITERATIONS

0 ANSWERS

SEARCH TIME: 00.00.01

L6 0 SEA SUB=L3 SSS FUL L4

=> d his

(FILE 'HOME' ENTERED AT 18:12:29 ON 11 NOV 2008)

FILE 'REGISTRY' ENTERED AT 18:12:36 ON 11 NOV 2008

L1 STRUCTURE UPLOADED

L2 10 S L1 SAM

L3 102 S L1 FULL

FILE 'STNGUIDE' ENTERED AT 18:13:28 ON 11 NOV 2008

FILE 'REGISTRY' ENTERED AT 18:14:27 ON 11 NOV 2008

L4 STRUCTURE UPLOADED

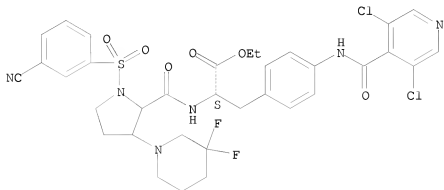
L5 0 S L4 SAM SUB=L3

L6 0 S L4 FULL SUB=L3

=> d scan 13

L3 102 ANSWERS REGISTRY COPYRIGHT 2008 ACS on STN
IN L-Phenylalanine, 1-[(3-cyanophenyl)sulfonyl]-3-(3,3-difluoro-1-piperidinyl)propyl-4-[[(3,5-dichloro-4-pyridinyl)carbonyl]amino]-, ethyl ester (9CI)
MF C34 H34 Cl2 F2 N6 O6 S

Absolute stereochemistry.

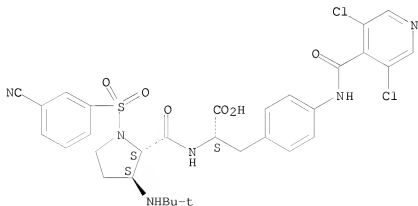


PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

HOW MANY MORE ANSWERS DO YOU WISH TO SCAN? (1):1

L3 102 ANSWERS REGISTRY COPYRIGHT 2008 ACS on STN
IN L-Phenylalanine, (3S)-1-[(3-cyanophenyl)sulfonyl]-3-[(1,1-dimethylethyl)amino]-L-propyl-4-[[(3,5-dichloro-4-pyridinyl)carbonyl]amino]-, monosodium salt (9CI)
MF C31 H32 Cl2 N6 O6 S . Na

Absolute stereochemistry.



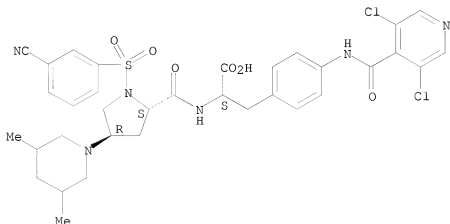
● Na

HOW MANY MORE ANSWERS DO YOU WISH TO SCAN? (1):1

L3 102 ANSWERS REGISTRY COPYRIGHT 2008 ACS on STN
IN L-Phenylalanine, (4R)-1-[(3-cyanophenyl)sulfonyl]-4-(3,5-dimethyl-1-piperidinyl)-L-prolyl-4-[[[(3,5-dichloro-4-pyridinyl)carbonyl]amino]-, mono(trifluoroacetate) (9CI)
MF C34 H36 Cl2 N6 O6 S . C2 H F3 O2

CM 1

Absolute stereochemistry.



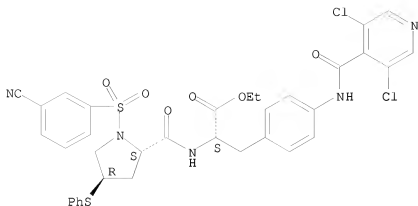
CM 2



HOW MANY MORE ANSWERS DO YOU WISH TO SCAN? (1):1

L3 102 ANSWERS REGISTRY COPYRIGHT 2008 ACS on STN
IN L-Phenylalanine, (4R)-1-[(3-cyanophenyl)sulfonyl]-4-(phenylthio)-L-prolyl-4-[[[(3,5-dichloro-4-pyridinyl)carbonyl]amino]-, ethyl ester (9CI)
MF C35 H31 Cl2 N5 O6 S2

Absolute stereochemistry.



PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

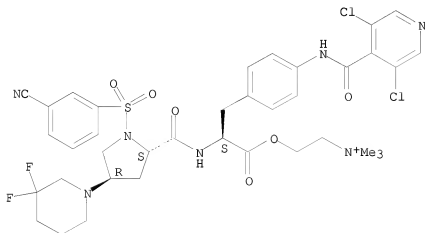
HOW MANY MORE ANSWERS DO YOU WISH TO SCAN? (1):1

L3 102 ANSWERS REGISTRY COPYRIGHT 2008 ACS on STN

IN L-Phenylalanine, (4R)-1-[(3-cyanophenyl)sulfonyl]-4-(3,3-difluoro-1-piperidinyl)-L-prolyl-4-[[[(3,5-dichloro-4-pyridinyl)carbonyl]amino]-, 2-(trimethylammonio)ethyl ester (9CI)

MF C37 H42 Cl2 F2 N7 O6 S

Absolute stereochemistry.



HOW MANY MORE ANSWERS DO YOU WISH TO SCAN? (1):1

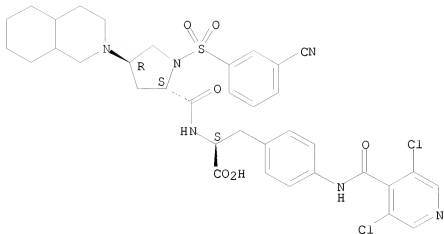
L3 102 ANSWERS REGISTRY COPYRIGHT 2008 ACS on STN

IN L-Phenylalanine, (4R)-1-[(3-cyanophenyl)sulfonyl]-4-(octahydro-2(1H)-isoquinolinyl)-L-prolyl-4-[[[(3,5-dichloro-4-pyridinyl)carbonyl]amino]- (9CI)

MF C36 H38 Cl2 N6 O6 S

CI COM

Absolute stereochemistry.



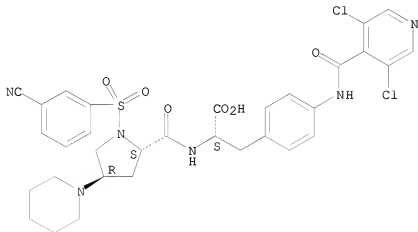
PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

HOW MANY MORE ANSWERS DO YOU WISH TO SCAN? (1):1

L3 102 ANSWERS REGISTRY COPYRIGHT 2008 ACS on STN
 IN L-Phenylalanine, (4R)-1-[(3-cyanophenyl)sulfonyl]-4-(1-piperidinyl)-L-
 prolyl-4-[[[(3,5-dichloro-4-pyridinyl)carbonyl]amino]-,
 mono(trifluoroacetate) (9CI)
 MF C32 H32 Cl2 N6 O6 S . C2 H F3 O2

CM 1

Absolute stereochemistry.



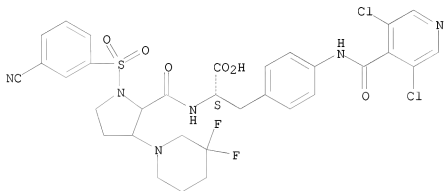
CM 2



HOW MANY MORE ANSWERS DO YOU WISH TO SCAN? (1):1

L3 102 ANSWERS REGISTRY COPYRIGHT 2008 ACS on STN
 IN L-Phenylalanine, 1-[(3-cyanophenyl)sulfonyl]-3-(3,3-difluoro-1-piperidinyl)prolyl-4-[[[(3,5-dichloro-4-pyridinyl)carbonyl]amino]- (9CI)
 MF C32 H30 Cl2 F2 N6 O6 S

Absolute stereochemistry.

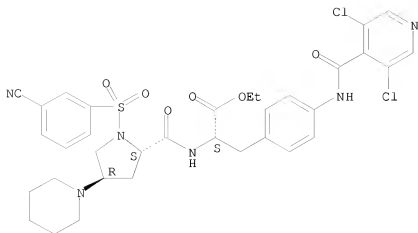


PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

HOW MANY MORE ANSWERS DO YOU WISH TO SCAN? (1):1

L3 102 ANSWERS REGISTRY COPYRIGHT 2008 ACS on STN
 IN L-Phenylalanine, (4R)-1-[(3-cyanophenyl)sulfonyl]-4-(1-piperidinyl)-L-prolyl-4-[[[(3,5-dichloro-4-pyridinyl)carbonyl]amino]-, ethyl ester (9CI)
 MF C34 H36 Cl2 N6 O6 S
 CI COM

Absolute stereochemistry.

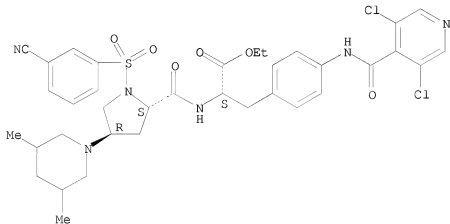


PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

HOW MANY MORE ANSWERS DO YOU WISH TO SCAN? (1):1

L3 102 ANSWERS REGISTRY COPYRIGHT 2008 ACS on STN
 IN L-Phenylalanine, (4R)-1-[(3-cyanophenyl)sulfonyl]-4-(3,5-dimethyl-1-piperidinyl)-L-prolyl-4-[[[(3,5-dichloro-4-pyridinyl)carbonyl]amino]-ethyl ester (9CI)
 MF C36 H40 Cl2 N6 O6 S
 CI COM

Absolute stereochemistry.

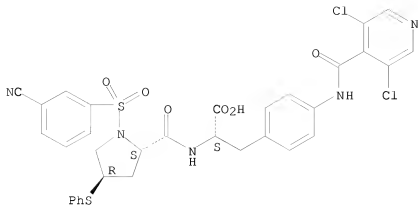


PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

HOW MANY MORE ANSWERS DO YOU WISH TO SCAN? (1):1

L3 102 ANSWERS REGISTRY COPYRIGHT 2008 ACS on STN
 IN L-Phenylalanine, (4R)-1-[(3-cyanophenyl)sulfonyl]-4-(phenylthio)-L-prolyl-4-[[[(3,5-dichloro-4-pyridinyl)carbonyl]amino]- (9CI)
 MF C33 H27 Cl2 N5 O6 S2

Absolute stereochemistry.

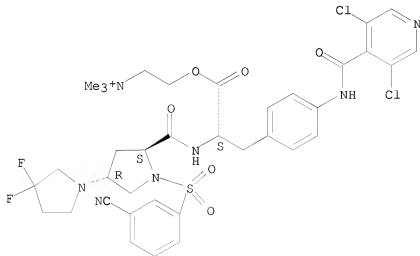


PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

HOW MANY MORE ANSWERS DO YOU WISH TO SCAN? (1):1

L3 102 ANSWERS REGISTRY COPYRIGHT 2008 ACS ON STN
 IN L-Phenylalanine, (4R)-1-[(3-cyanophenyl)sulfonyl]-4-[(3,3-difluoro-1-pyrrolidiny)-L-prolyl-4-[[[(3,5-dichloro-4-pyridinyl)carbonyl]amino]-2-(trimethylammonio)ethyl ester (9CI)
 MF C36 H40 Cl2 F2 N7 O6 S

Absolute stereochemistry.



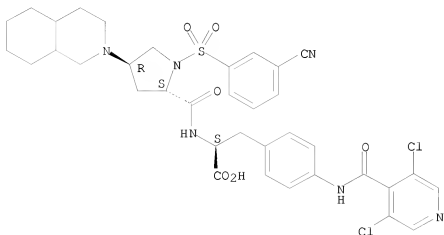
HOW MANY MORE ANSWERS DO YOU WISH TO SCAN? (1):1

L3 102 ANSWERS REGISTRY COPYRIGHT 2008 ACS ON STN
 IN L-Phenylalanine, (4R)-1-[(3-cyanophenyl)sulfonyl]-4-(octahydro-2(1H)-isoquinoliny)-L-prolyl-4-[[[(3,5-dichloro-4-pyridinyl)carbonyl]amino]-mono(trifluoroacetate) (9CI)

MF C36 H38 Cl2 N6 O6 S . C2 H F3 O2

CM 1

Absolute stereochemistry.



CM 2



HOW MANY MORE ANSWERS DO YOU WISH TO SCAN? (1):1

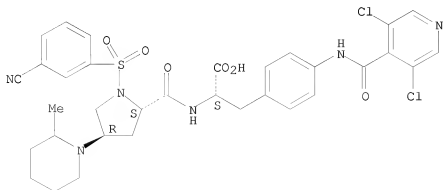
L3 102 ANSWERS REGISTRY COPYRIGHT 2008 ACS on STN

IN L-Phenylalanine, (4R)-1-[(3-cyanophenyl)sulfonyl]-4-(2-methyl-1-piperidinyl)-L-prolyl-4-[[3,5-dichloro-4-pyridinyl]carbonyl]amino]- (9CI)

MF C33 H34 Cl2 N6 O6 S

CI COM

Absolute stereochemistry.



PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

HOW MANY MORE ANSWERS DO YOU WISH TO SCAN? (1):0

=> fil caplus

COST IN U.S. DOLLARS

SINCE FILE

TOTAL

ENTRY

SESSION

FULL ESTIMATED COST

44.86

223.55

FILE 'CAPLUS' ENTERED AT 18:18:15 ON 11 NOV 2008

USE IS SUBJECT TO THE TERMS OF YOUR STN CUSTOMER AGREEMENT.

PLEASE SEE "HELP USAGETERMS" FOR DETAILS.

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FILE COVERS 1907 - 11 Nov 2008 VOL 149 ISS 20

FILE LAST UPDATED: 10 Nov 2008 (20081110/ED)

Caplus now includes complete International Patent Classification (IPC) reclassification data for the second quarter of 2008.

Effective October 17, 2005, revised CAS Information Use Policies apply. They are available for your review at:

<http://www.cas.org/legal/infopolicy.html>

'OBI' IS DEFAULT SEARCH FIELD FOR 'CAPLUS' FILE

=> d his

(FILE 'HOME' ENTERED AT 18:12:29 ON 11 NOV 2008)

FILE 'REGISTRY' ENTERED AT 18:12:36 ON 11 NOV 2008

L1 STRUCTURE UPLOADED

L2 10 S L1 SAM

L3 102 S L1 FULL

FILE 'STNGUIDE' ENTERED AT 18:13:28 ON 11 NOV 2008

FILE 'REGISTRY' ENTERED AT 18:14:27 ON 11 NOV 2008

L4 STRUCTURE UPLOADED

L5 0 S L4 SAM SUB=L3

L6 0 S L4 FULL SUB=L3

FILE 'CAPLUS' ENTERED AT 18:18:15 ON 11 NOV 2008

=> s 13

L7 4 L3

=> d ti 1-4

L7 ANSWER 1 OF 4 CAPLUS COPYRIGHT 2008 ACS on STN
 TI Preparation of prolyl peptide derivatives as VLA-4 antagonists

L7 ANSWER 2 OF 4 CAPLUS COPYRIGHT 2008 ACS on STN
 TI Preparation of dipeptide derivatives as VLA-4 antagonists

L7 ANSWER 3 OF 4 CAPLUS COPYRIGHT 2008 ACS on STN
 TI Preparation of prolylphenylalanine derivatives as VLA-4 antagonists

L7 ANSWER 4 OF 4 CAPLUS COPYRIGHT 2008 ACS on STN
 TI Preparation of N-arylsulfonyl aza-bicyclic derivatives as potent cell adhesion inhibitors

=> s US20070179190/pn
 L8 1 US20070179190/PN

=> d ti

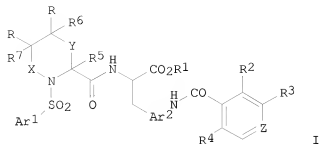
L8 ANSWER 1 OF 1 CAPLUS COPYRIGHT 2008 ACS on STN
 TI Preparation of prolylphenylalanine derivatives as VLA-4 antagonists

=> d ibib abs hitstr l7 4

L7 ANSWER 4 OF 4 CAPLUS COPYRIGHT 2008 ACS on STN
 ACCESSION NUMBER: 2003:23531 CAPLUS
 DOCUMENT NUMBER: 138:90079
 TITLE: Preparation of N-arylsulfonyl aza-bicyclic derivatives as potent cell adhesion inhibitors
 INVENTOR(S): Lin, Linus S.; Doherty, George; Shah, Shrenik K.; Chang, Linda L.; Hagmann, William K.; Mumford, Richard A.
 PATENT ASSIGNEE(S): Merck & Co., Inc., USA
 SOURCE: U.S. Pat. Appl. Publ., 31 pp.
 CODEN: USXXCO
 DOCUMENT TYPE: Patent
 LANGUAGE: English
 FAMILY ACC. NUM. COUNT: 1
 PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
US 20030008861	A1	20030109	US 2002-96607	20020313
US 6855708	B2	20050215		
PRIORITY APPLN. INFO.:			US 2001-277233P	P 20010320
OTHER SOURCE(S):	MARPAT	138:90079		

GI



AB Compds. I [R2 is an (un)substituted cycloalkyl or heterocyclyl ring; R1 = H, alkyl, arylalkyl; R2, R4 = halo, alkyl, alkoxy; R3 = H, OH, MeO, NH2; Z = N or N:O; Ar1 = (un)substituted Ph, pyridyl, pyridazinyl, pyrimidinyl, pyrazinyl, or triazinyl; Ar2 = 1,4-phenylene or 2,5-pyridylene; X, Y = (CH2)0-2; R5 = H, alkyl; R6, R7 = H, alkyl, OH, alkoxy, carboxy, amino, sulfonylamino, etc.] or their pharmaceutically-acceptable salts were prepared as antagonists of VLA-4 and/or $\alpha 4\beta 7$ and as such are useful in the inhibition or prevention of cell adhesion and cell-adhesion mediated pathologies. Thus, N-[N-(3,5-dichlorobenzene-sulfonyl)octahydroisindole-1-carbonyl]-4-[(3,5-dichloroisonicotinoyl)amino]-L-phenylalanine was prepared by coupling of N-(3,5-dichlorobenzene-sulfonyl)octahydroisindole-1-carboxylic acid chloride with 4-[(3,5-dichloroisonicotinoyl)amino]-L-phenylalanine tert-Bu ester (syntheses given), followed by separation of diastereomers and ester cleavage.

IT 483973-78-0P

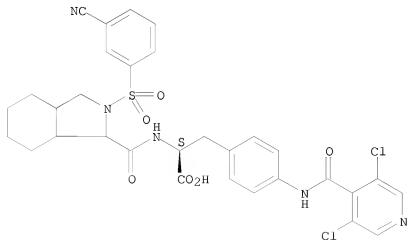
RL: PAC (Pharmacological activity); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)

(preparation of N-arylsulfonyl heteroaroyl amino acid derivs. as cell adhesion inhibitors)

RN 483973-78-0 CAPLUS

CN L-Phenylalanine, N-[[2-[(3-cyanophenyl)sulfonyl]octahydro-1H-isindol-1-yl]carbonyl]-4-[(3,5-dichloro-4-pyridinyl)carbonyl]amino]- (CA INDEX NAME)

Absolute stereochemistry.



RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

=> d his

(FILE 'HOME' ENTERED AT 18:12:29 ON 11 NOV 2008)

FILE 'REGISTRY' ENTERED AT 18:12:36 ON 11 NOV 2008

L1 STRUCTURE UPLOADED
L2 10 S L1 SAM
L3 102 S L1 FULL

FILE 'STNGUIDE' ENTERED AT 18:13:28 ON 11 NOV 2008

FILE 'REGISTRY' ENTERED AT 18:14:27 ON 11 NOV 2008

L4 STRUCTURE UPLOADED
L5 0 S L4 SAM SUB=L3
L6 0 S L4 FULL SUB=L3

FILE 'CAPLUS' ENTERED AT 18:18:15 ON 11 NOV 2008

L7 4 S L3
L8 1 S US20070179190/PN

=> fil medline biosis embase

COST IN U.S. DOLLARS	SINCE FILE ENTRY	TOTAL SESSION
FULL ESTIMATED COST	10.81	234.36

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CA SUBSCRIBER PRICE	-0.80	-0.80

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=> s l3

L9 0 L3

=> fil stng

COST IN U.S. DOLLARS	SINCE FILE ENTRY	TOTAL SESSION
FULL ESTIMATED COST	9.08	243.44

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CA SUBSCRIBER PRICE	0.00	-0.80

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COST IN U.S. DOLLARS	SINCE FILE ENTRY	TOTAL SESSION
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FULL ESTIMATED COST	0.18	243.62
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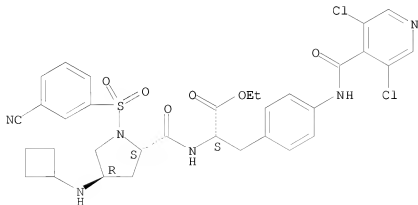
<http://www.cas.org/support/stngen/stndoc/properties.html>

=> d scan 13

L3 102 ANSWERS REGISTRY COPYRIGHT 2008 ACS ON STN
 IN L-Phenylalanine, (4R)-1-[(3-cyanophenyl)sulfonyl]-4-(cyclobutylamino)-L-prolyl-4-[[[3,5-dichloro-4-pyridinyl)carbonyl]amino]-, ethyl ester, monomethanesulfonate (9CI)
 MF C33 H34 Cl2 N6 O6 S . C H4 O3 S

CM 1

Absolute stereochemistry.



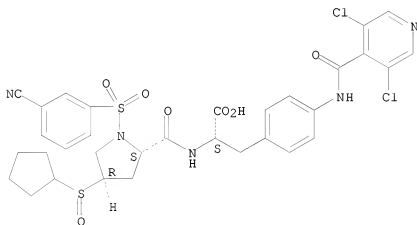
CM 2



HOW MANY MORE ANSWERS DO YOU WISH TO SCAN? (1):102

L3 102 ANSWERS REGISTRY COPYRIGHT 2008 ACS ON STN
 IN L-Phenylalanine, (4R)-1-[(3-cyanophenyl)sulfonyl]-4-(cyclopentylsulfinyl)-
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 MF C32 H31 Cl2 N5 O7 S2

Absolute stereochemistry.

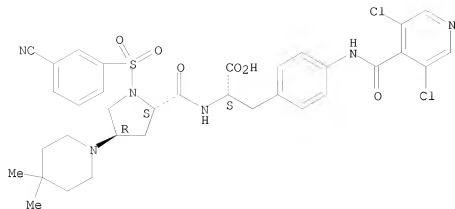


PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

L3 102 ANSWERS REGISTRY COPYRIGHT 2008 ACS ON STN
 IN L-Phenylalanine, (4R)-1-[(3-cyanophenyl)sulfonyl]-4-(4,4-dimethyl-1-piperidinyl)-L-prolyl-4-[[[(3,5-dichloro-4-pyridinyl)carbonyl]amino]-, mono(trifluoroacetate) (9CI)
 MF C34 H36 Cl2 N6 O6 S . C2 H F3 O2

CM 1

Absolute stereochemistry.

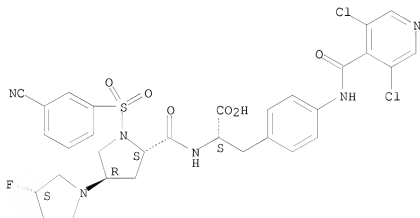


CM 2



L3 102 ANSWERS REGISTRY COPYRIGHT 2008 ACS on STN
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 (9CI)
 MF C31 H29 Cl2 F N6 O6 S

Absolute stereochemistry.



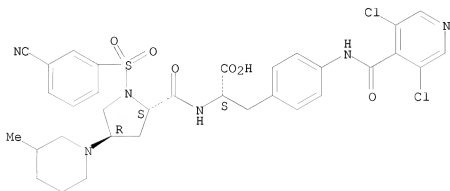
PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

L3 102 ANSWERS REGISTRY COPYRIGHT 2008 ACS on STN

IN L-Phenylalanine, (4R)-1-[(3-cyanophenyl)sulfonyl]-4-(3-methyl-1-piperidinyl)-L-prolyl-4-[[(3,5-dichloro-4-pyridinyl)carbonyl]amino]-, mono(trifluoroacetate) (9CI)
 MF C33 H34 Cl2 N6 O6 S . C2 H F3 O2

CM 1

Absolute stereochemistry.

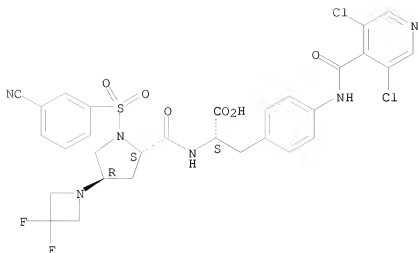


CM 2



L3 102 ANSWERS REGISTRY COPYRIGHT 2008 ACS on STN
 IN L-Phenylalanine, (4R)-1-[(3-cyanophenyl)sulfonyl]-4-(3,3-difluoro-1-azetidiny)-L-prolyl-4-[[(3,5-dichloro-4-pyridinyl)carbonyl]amino]- (9CI)
 MF C30 H26 Cl2 F2 N6 O6 S

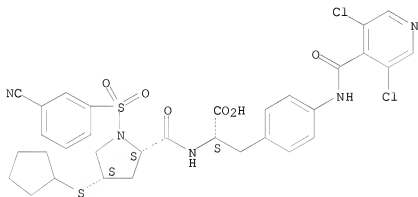
Absolute stereochemistry.



PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

L3 102 ANSWERS REGISTRY COPYRIGHT 2008 ACS on STN
 IN L-Phenylalanine, (4S)-1-[(3-cyanophenyl)sulfonyl]-4-[(cyclopentylthio)-L-prolyl-4-[[[(3,5-dichloro-4-pyridinyl)carbonyl]amino]- (9CI)
 MF C32 H31 Cl2 N5 O6 S2

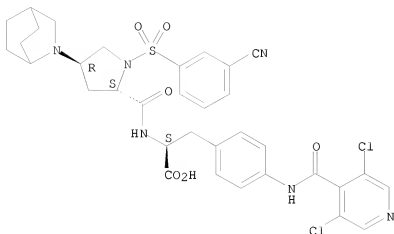
Absolute stereochemistry.



PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

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 IN L-Phenylalanine, (4R)-4-(2-azabicyclo[2.2.2]oct-2-yl)-1-[(3-cyanophenyl)sulfonyl]-L-prolyl-4-[[[(3,5-dichloro-4-pyridinyl)carbonyl]amino]- (9CI)
 MF C34 H34 Cl2 N6 O6 S
 CI COM

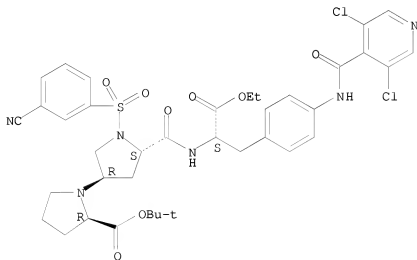
Absolute stereochemistry.



PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

L3 102 ANSWERS REGISTRY COPYRIGHT 2008 ACS on STN
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 MF C38 H42 Cl2 N6 O8 S

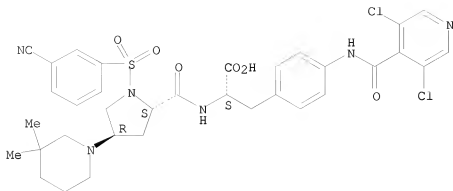
Absolute stereochemistry.



PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

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 IN L-Phenylalanine, (4R)-1-[(3-cyanophenyl)sulfonyl]-4-(3,3-dimethyl-1-piperidinyl)-L-prolyl-4-[[[3,5-dichloro-4-pyridinyl)carbonyl]amino]- (9CI)
 MF C34 H36 Cl2 N6 O6 S
 CI COM

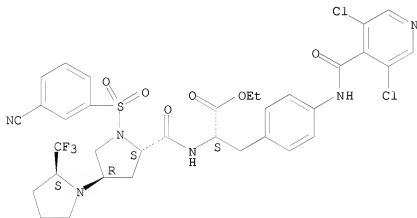
Absolute stereochemistry.



PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

L3 102 ANSWERS REGISTRY COPYRIGHT 2008 ACS on STN
 IN L-Phenylalanine, (4R)-1-[(3-cyanophenyl)sulfonyl]-4-[(2S)-2-(trifluoromethyl)-1-pyrrolidinyl]-L-prolyl-4-[[3,5-dichloro-4-pyridinyl)carbonylamino]-, ethyl ester (9CI)
 MF C34 H33 Cl2 F3 N6 O6 S

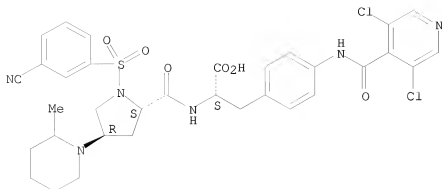
Absolute stereochemistry.



PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

L3 102 ANSWERS REGISTRY COPYRIGHT 2008 ACS on STN
 IN L-Phenylalanine, (4R)-1-[(3-cyanophenyl)sulfonyl]-4-(2-methyl-1-piperidinyl)-L-prolyl-4-[[3,5-dichloro-4-pyridinyl)carbonylamino]- (9CI)
 MF C33 H34 Cl2 N6 O6 S
 CI COM

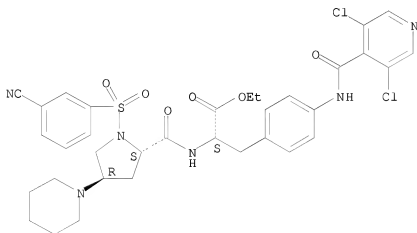
Absolute stereochemistry.



PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

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 IN L-Phenylalanine, (4R)-1-[(3-cyanophenyl)sulfonyl]-4-(1-piperidinyl)-L-prolyl-4-[[(3,5-dichloro-4-pyridinyl)carbonylamino]-, ethyl ester (9CI)
 MF C34 H36 Cl2 N6 O6 S
 CI COM

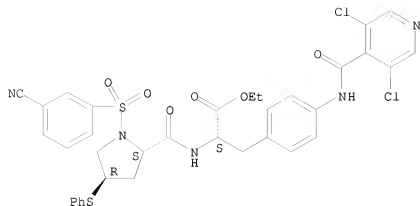
Absolute stereochemistry.



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 IN L-Phenylalanine, (4R)-1-[(3-cyanophenyl)sulfonyl]-4-(phenylthio)-L-prolyl-4-[[(3,5-dichloro-4-pyridinyl)carbonylamino]-, ethyl ester (9CI)
 MF C35 H31 Cl2 N5 O6 S2

Absolute stereochemistry.

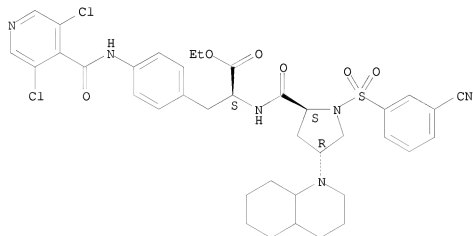


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 IN L-Phenylalanine, (4R)-1-[(3-cyanophenyl)sulfonyl]-4-(octahydro-1(2H)-quinoliny)-L-prolyl-4-[[[(3,5-dichloro-4-pyridinyl)carbonylamino]-, ethyl ester, mono(trifluoroacetate) (9CI)
 MF C38 H42 Cl2 N6 O6 S . C2 H F3 O2

CM 1

Absolute stereochemistry.

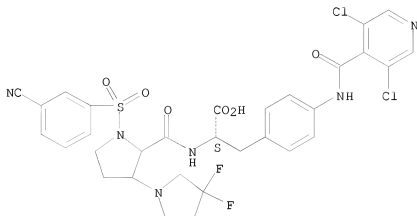


CM 2



L3 102 ANSWERS REGISTRY COPYRIGHT 2008 ACS on STN
 IN L-Phenylalanine, 1-[(3-cyanophenyl)sulfonyl]-3-(3,3-difluoro-1-pyrrolidinyl)-L-prolyl-4-[[[(3,5-dichloro-4-pyridinyl)carbonyl]amino]-
 (9CI)
 MF C31 H28 Cl2 F2 N6 O6 S

Absolute stereochemistry.

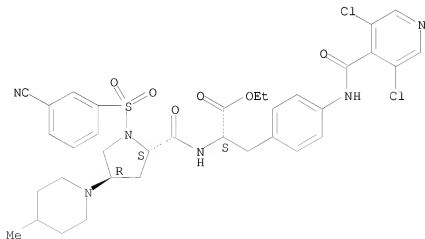


PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

L3 102 ANSWERS REGISTRY COPYRIGHT 2008 ACS on STN
 IN L-Phenylalanine, (4R)-1-[(3-cyanophenyl)sulfonyl]-4-[(4-methyl-1-piperidinyl)-L-prolyl-4-[[[(3,5-dichloro-4-pyridinyl)carbonyl]amino]-,
 ethyl ester, mono(trifluoroacetate) (9CI)
 MF C35 H38 Cl2 N6 O6 S . C2 H F3 O2

CM 1

Absolute stereochemistry.

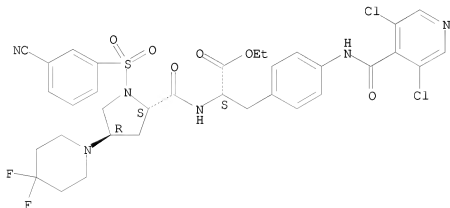


CM 2



L3 102 ANSWERS REGISTRY COPYRIGHT 2008 ACS on STN
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MF C34 H34 Cl2 F2 N6 O6 S

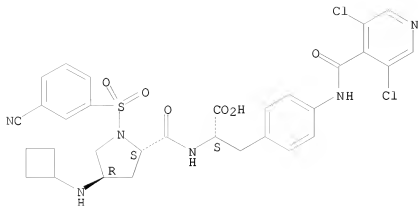
Absolute stereochemistry.



PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

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L3 102 ANSWERS  REGISTRY  COPYRIGHT 2008 ACS on STN
IN L-Phenylalanine, (4R)-1-[(3-cyanophenyl)sulfonyl]-4-(cyclobutylamino)-L-
MF prolyl-4-[[[3,5-dichloro-4-pyridinyl]carbonyl]amino]- (9CI)
CI C31 H30 Cl2 N6 O6 S
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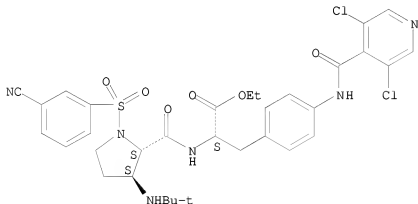
Absolute stereochemistry.



PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

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 IN L-Phenylalanine, (3S)-1-[(3-cyanophenyl)sulfonyl]-3-[(1,1-dimethylethyl)amino]-L-prolyl-4-[(3,5-dichloro-4-pyridinyl)carbonylamino]-, ethyl ester (9CI)
 MF C33 H36 Cl2 N6 O6 S

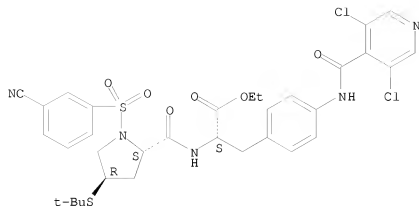
Absolute stereochemistry.



PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

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 MF C33 H35 Cl2 N5 O6 S2

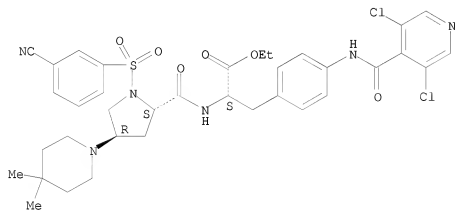
Absolute stereochemistry.



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 MF C36 H40 Cl2 N6 O6 S
 CI COM

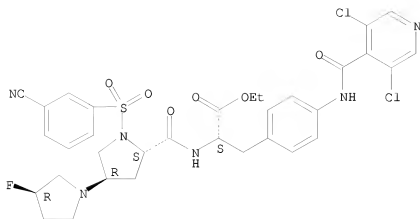
Absolute stereochemistry.



PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

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 MF C33 H33 Cl2 F N6 O6 S

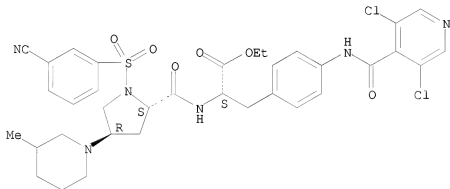
Absolute stereochemistry.



PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

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 MF C35 H38 Cl2 N6 O6 S
 CI COM

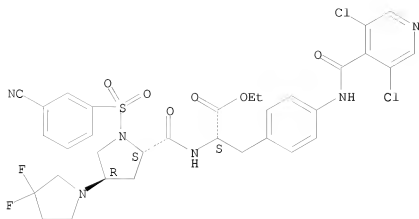
Absolute stereochemistry.



PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

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 MF C33 H32 Cl2 F2 N6 O6 S

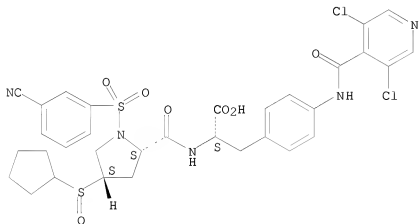
Absolute stereochemistry.



PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

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 IN L-Phenylalanine, (4S)-1-[(3-cyanophenyl)sulfonyl]-4-(cyclopentylsulfinyl)-
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 MF C32 H31 Cl2 N5 O7 S2

Absolute stereochemistry.

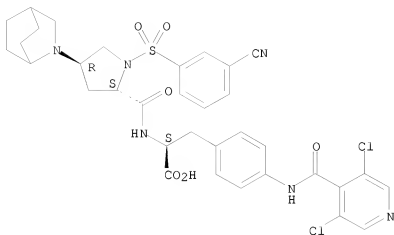


PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

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 MF C34 H34 Cl2 N6 O6 S . C2 H F3 O2

CM 1

Absolute stereochemistry.

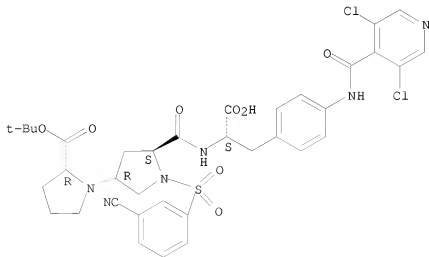


CM 2



L3 102 ANSWERS REGISTRY COPYRIGHT 2008 ACS on STN
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 MF C36 H38 Cl2 N6 O8 S

Absolute stereochemistry.

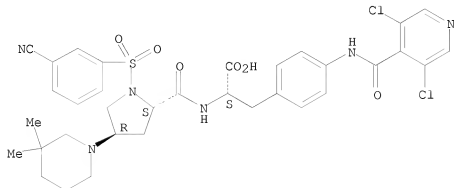


PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

L3 102 ANSWERS REGISTRY COPYRIGHT 2008 ACS on STN
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 MF C34 H36 Cl2 N6 O6 S . C2 H F3 O2

CM 1

Absolute stereochemistry.

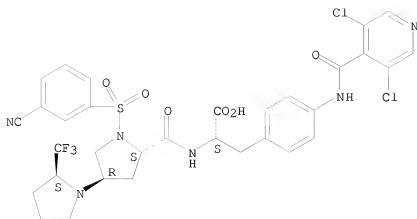


CM 2



L3 102 ANSWERS REGISTRY COPYRIGHT 2008 ACS on STN
 IN L-Phenylalanine, (4R)-1-[(3-cyanophenyl)sulfonyl]-4-[(2S)-2-(trifluoromethyl)-1-pyrrolidinyl]-L-prolyl-4-[[[(3,5-dichloro-4-pyridinyl)carbonyl]amino]- (9CI)
 MF C32 H29 Cl2 F3 N6 O6 S

Absolute stereochemistry.

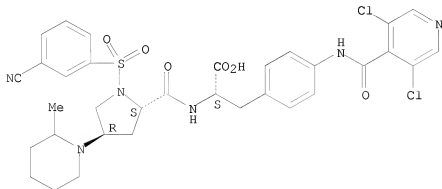


PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

L3 102 ANSWERS REGISTRY COPYRIGHT 2008 ACS on STN
 IN L-Phenylalanine, (4R)-1-[(3-cyanophenyl)sulfonyl]-4-(2-methyl-1-piperidinyl)-L-prolyl-4-[[3,5-dichloro-4-pyridinyl)carbonyl]amino]-, mono(trifluoroacetate) (9CI)
 MF C33 H34 Cl2 N6 O6 S . C2 H F3 O2

CM 1

Absolute stereochemistry.



CM 2

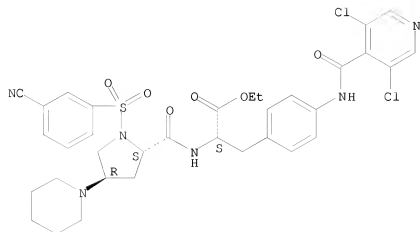


L3 102 ANSWERS REGISTRY COPYRIGHT 2008 ACS on STN
 IN L-Phenylalanine, (4R)-1-[(3-cyanophenyl)sulfonyl]-4-(1-piperidinyl)-L-prolyl-4-[[3,5-dichloro-4-pyridinyl)carbonyl]amino]-, ethyl ester,

mono(trifluoroacetate) (9CI)
 MF C34 H36 Cl2 N6 O6 S . C2 H F3 O2

CM 1

Absolute stereochemistry.

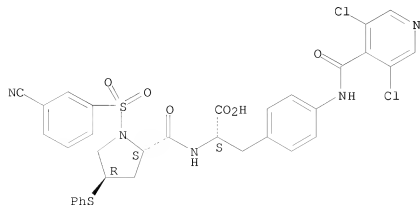


CM 2



L3 102 ANSWERS REGISTRY COPYRIGHT 2008 ACS on STN
 IN L-Phenylalanine, (4R)-1-[(3-cyanophenyl)sulfonyl]-4-(phenylthio)-L-prolyl-
 4-[(3,5-dichloro-4-pyridinyl)carbonyl]amino]- (9CI)
 MF C33 H27 Cl2 N5 O6 S2

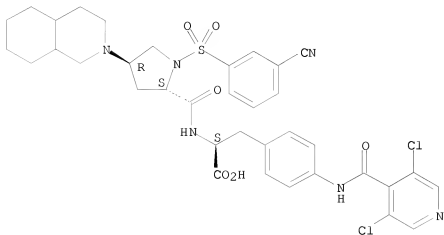
Absolute stereochemistry.



PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

L3 102 ANSWERS REGISTRY COPYRIGHT 2008 ACS on STN
IN L-Phenylalanine, (4R)-1-[(3-cyanophenyl)sulfonyl]-4-(octahydro-2(1H)-
isoquinolinyl)-L-prolyl-4-[[(3,5-dichloro-4-pyridinyl)carbonyl]amino]-
(9CI)
MF C36 H38 Cl2 N6 O6 S
CI COM

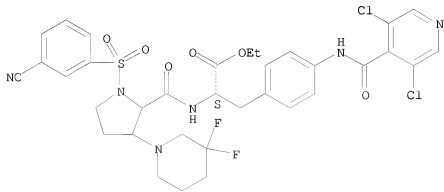
Absolute stereochemistry.



PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

L3 102 ANSWERS REGISTRY COPYRIGHT 2008 ACS on STN
IN L-Phenylalanine, 1-[(3-cyanophenyl)sulfonyl]-3-(3,3-difluoro-1-
piperidinyl)prolyl-4-[[(3,5-dichloro-4-pyridinyl)carbonyl]amino]-, ethyl
ester (9CI)
MF C34 H34 Cl2 F2 N6 O6 S

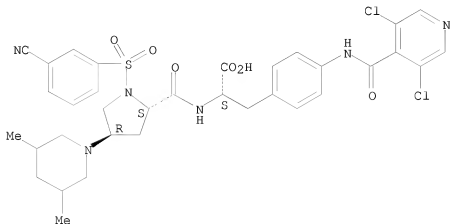
Absolute stereochemistry.



PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

L3 102 ANSWERS REGISTRY COPYRIGHT 2008 ACS on STN
 IN L-Phenylalanine, (4R)-1-[(3-cyanophenyl)sulfonyl]-4-(3,5-dimethyl-1-piperidinyl)-L-prolyl-4-[[(3,5-dichloro-4-pyridinyl)carbonyl]amino]- (9CI)
 MF C34 H36 Cl2 N6 O6 S
 CI COM

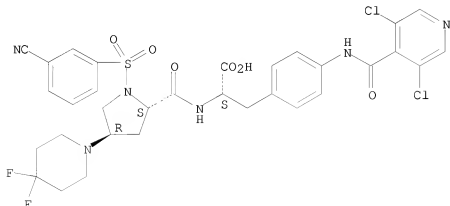
Absolute stereochemistry.



PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

L3 102 ANSWERS REGISTRY COPYRIGHT 2008 ACS on STN
 IN L-Phenylalanine, (4R)-1-[(3-cyanophenyl)sulfonyl]-4-(4,4-difluoro-1-piperidinyl)-L-prolyl-4-[[(3,5-dichloro-4-pyridinyl)carbonyl]amino]- (9CI)
 MF C32 H30 Cl2 F2 N6 O6 S

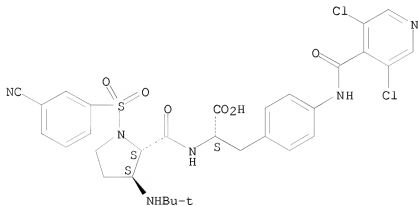
Absolute stereochemistry.



PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

L3 102 ANSWERS REGISTRY COPYRIGHT 2008 ACS on STN
 IN L-Phenylalanine, (3S)-1-[(3-cyanophenyl)sulfonyl]-3-[(1,1-dimethylethyl)amino]-L-prolyl-4-[[(3,5-dichloro-4-pyridinyl)carbonyl]amino]- (9CI)
 MF C31 H32 Cl2 N6 O6 S
 CI COM

Absolute stereochemistry.

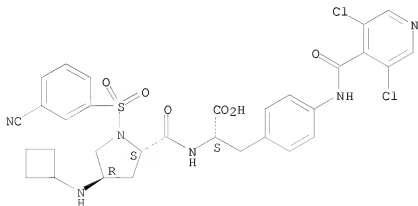


PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

L3 102 ANSWERS REGISTRY COPYRIGHT 2008 ACS on STN
 IN L-Phenylalanine, (4R)-1-[(3-cyanophenyl)sulfonyl]-4-(cyclobutylamino)-L-prolyl-4-[[(3,5-dichloro-4-pyridinyl)carbonyl]amino]-, monomethanesulfonate (9CI)
 MF C31 H30 Cl2 N6 O6 S . C H4 O3 S

CM 1

Absolute stereochemistry.

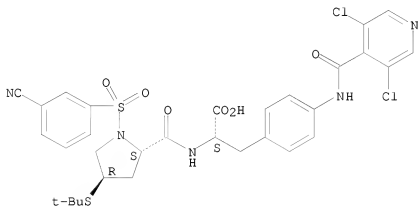


CM 2



L3 102 ANSWERS REGISTRY COPYRIGHT 2008 ACS on STN
 IN L-Phenylalanine, (4R)-1-[(3-cyanophenyl)sulfonyl]-4-[(1,1-dimethylethyl)thio]-L-prolyl-4-[[(3,5-dichloro-4-pyridinyl)carbonyl]amino]-
 (9CI)
 MF C31 H31 Cl2 N5 O6 S2

Absolute stereochemistry.

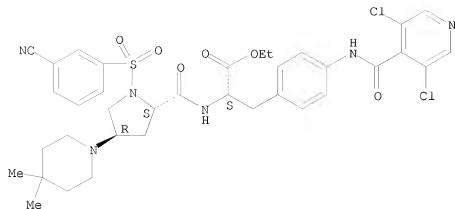


PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

L3 102 ANSWERS REGISTRY COPYRIGHT 2008 ACS on STN
 IN L-Phenylalanine, (4R)-1-[(3-cyanophenyl)sulfonyl]-4-(4,4-dimethyl-1-piperidinyl)-L-prolyl-4-[[(3,5-dichloro-4-pyridinyl)carbonyl]amino]-,
 ethyl ester, mono(trifluoroacetate) (9CI)
 MF C36 H40 Cl2 N6 O6 S . C2 H F3 O2

CM 1

Absolute stereochemistry.

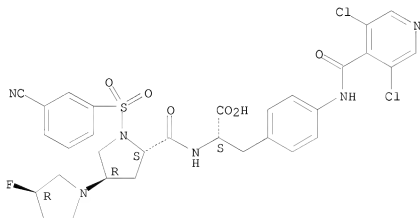


CM 2



L3 102 ANSWERS REGISTRY COPYRIGHT 2008 ACS on STN
 IN L-Phenylalanine, (4R)-1-[(3-cyanophenyl)sulfonyl]-4-[(3R)-3-fluoro-1-pyrrolidinyl]-L-prolyl-4-[[[3,5-dichloro-4-pyridinyl)carbonyl]amino]-(9CI)
 MF C31 H29 Cl2 F N6 O6 S

Absolute stereochemistry.



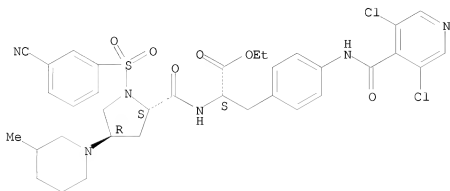
PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

L3 102 ANSWERS REGISTRY COPYRIGHT 2008 ACS on STN

IN L-Phenylalanine, (4R)-1-[(3-cyanophenyl)sulfonyl]-4-(3-methyl-1-piperidinyl)-L-prolyl-4-[[(3,5-dichloro-4-pyridinyl)carbonyl]amino]-ethyl ester, mono(trifluoroacetate) (9CI)
 MF C35 H38 Cl2 N6 O6 S . C2 H F3 O2

CM 1

Absolute stereochemistry.

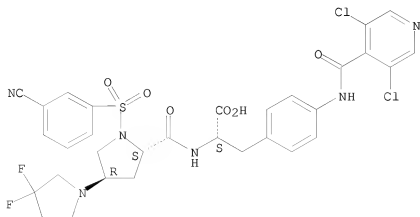


CM 2



L3 102 ANSWERS REGISTRY COPYRIGHT 2008 ACS on STN
 IN L-Phenylalanine, (4R)-1-[(3-cyanophenyl)sulfonyl]-4-(3,3-difluoro-1-pyrrolidiny)-L-prolyl-4-[[(3,5-dichloro-4-pyridinyl)carbonyl]amino]-ethyl ester, mono(trifluoroacetate) (9CI)
 MF C31 H28 Cl2 F2 N6 O6 S

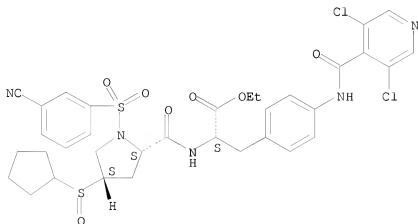
Absolute stereochemistry.



PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

L3 102 ANSWERS REGISTRY COPYRIGHT 2008 ACS on STN
IN L-Phenylalanine, (4S)-1-[(3-cyanophenyl)sulfonyl]-4-(cyclopentylsulfinyl)-
L-prolyl-4-[[[(3,5-dichloro-4-pyridinyl)carbonyl]amino]-, ethyl ester (9CI)
MF C34 H35 Cl2 N5 O7 S2

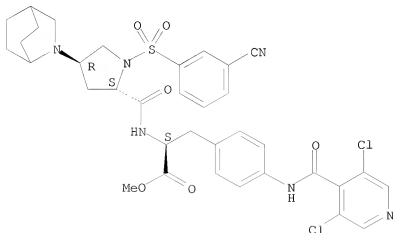
Absolute stereochemistry.



PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

L3 102 ANSWERS REGISTRY COPYRIGHT 2008 ACS on STN
IN L-Phenylalanine, (4R)-4-(2-azabicyclo[2.2.2]oct-2-yl)-1-[(3-cyanophenyl)sulfonyl]-L-prolyl-4-[[[(3,5-dichloro-4-pyridinyl)carbonyl]amino]-, methyl ester (9CI)
MF C35 H36 Cl2 N6 O6 S
CI COM

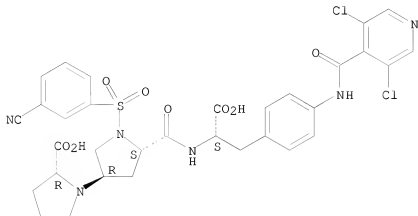
Absolute stereochemistry.



PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

L3 102 ANSWERS REGISTRY COPYRIGHT 2008 ACS on STN
IN L-Phenylalanine, (4R)-4-[(2R)-2-carboxy-1-pyrrolidinyl]-1-[(3-cyanophenyl)sulfonyl]-L-prolyl-4-[[[(3,5-dichloro-4-pyridinyl)carbonylamino]- (9CI)
MF C32 H30 Cl2 N6 O8 S

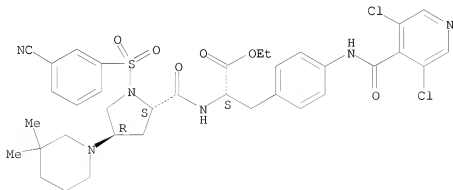
Absolute stereochemistry.



PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

L3 102 ANSWERS REGISTRY COPYRIGHT 2008 ACS on STN
IN L-Phenylalanine, (4R)-1-[(3-cyanophenyl)sulfonyl]-4-(3,3-dimethyl-1-piperidinyl)-L-prolyl-4-[[[(3,5-dichloro-4-pyridinyl)carbonylamino]-, ethyl ester (9CI)
MF C36 H40 Cl2 N6 O6 S
CI COM

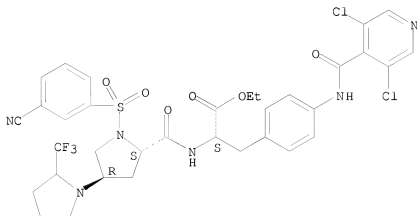
Absolute stereochemistry.



PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

L3 102 ANSWERS REGISTRY COPYRIGHT 2008 ACS on STN
 IN L-Phenylalanine, (4R)-1-[(3-cyanophenyl)sulfonyl]-4-[2-(trifluoromethyl)-1-pyrrolidinyl]-L-prolyl-4-[[(3,5-dichloro-4-pyridinyl)carbonyl]amino]-, ethyl ester (9CI)
 MF C34 H33 Cl2 F3 N6 O6 S

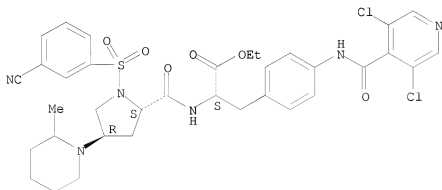
Absolute stereochemistry.



PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

L3 102 ANSWERS REGISTRY COPYRIGHT 2008 ACS on STN
 IN L-Phenylalanine, (4R)-1-[(3-cyanophenyl)sulfonyl]-4-(2-methyl-1-piperidinyl)-L-prolyl-4-[[(3,5-dichloro-4-pyridinyl)carbonyl]amino]-, ethyl ester (9CI)
 MF C35 H38 Cl2 N6 O6 S
 CI COM

Absolute stereochemistry.

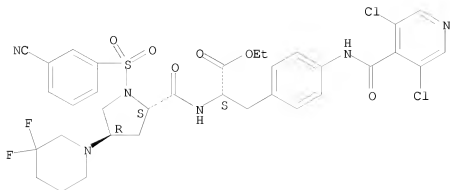


PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

L3 102 ANSWERS REGISTRY COPYRIGHT 2008 ACS on STN
 IN L-Phenylalanine, (4R)-1-[(3-cyanophenyl)sulfonyl]-4-(3,3-difluoro-1-piperidinyl)-L-prolyl-4-[[(3,5-dichloro-4-pyridinyl)carbonyl]amino]-, ethyl ester (9CI)

ethyl ester (9CI)
 MF C34 H34 Cl2 F2 N6 O6 S

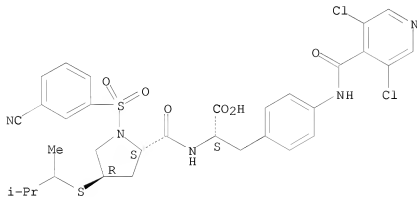
Absolute stereochemistry.



PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

L3 102 ANSWERS REGISTRY COPYRIGHT 2008 ACS on STN
 IN L-Phenylalanine, (4R)-1-[(3-cyanophenyl)sulfonyl]-4-[(1,2-dimethylpropyl)thio]-L-prolyl-4-[[[(3,5-dichloro-4-pyridinyl)carbonyl]amino]- (9CI)
 MF C32 H33 Cl2 N5 O6 S2

Absolute stereochemistry.

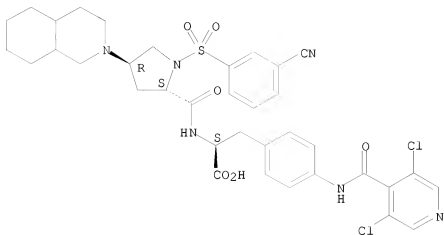


PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

L3 102 ANSWERS REGISTRY COPYRIGHT 2008 ACS on STN
 IN L-Phenylalanine, (4R)-1-[(3-cyanophenyl)sulfonyl]-4-(octahydro-2(1H)-isoquinolinyl)-L-prolyl-4-[[[(3,5-dichloro-4-pyridinyl)carbonyl]amino]-, mono(trifluoroacetate) (9CI)
 MF C36 H38 Cl2 N6 O6 S . C2 H F3 O2

CM 1

Absolute stereochemistry.

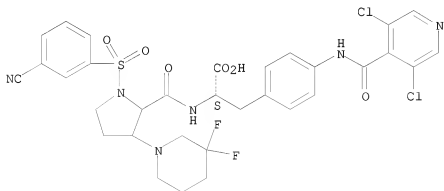


CM 2



L3 102 ANSWERS REGISTRY COPYRIGHT 2008 ACS on STN
 IN L-Phenylalanine, 1-[(3-cyanophenyl)sulfonyl]-3-(3,3-difluoro-1-
 piperidinyl)prolyl-4-[[[(3,5-dichloro-4-pyridinyl)carbonyl]amino]- (9CI)
 MF C32 H30 Cl2 F2 N6 O6 S

Absolute stereochemistry.

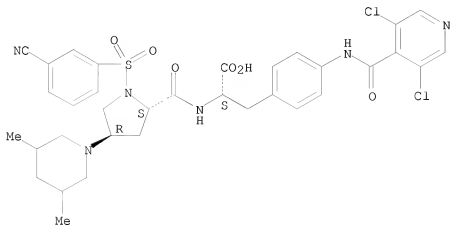


PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

L3 102 ANSWERS REGISTRY COPYRIGHT 2008 ACS on STN
 IN L-Phenylalanine, (4R)-1-[(3-cyanophenyl)sulfonyl]-4-(3,5-dimethyl-1-piperidinyl)-L-prolyl-4-[[[(3,5-dichloro-4-pyridinyl)carbonyl]amino]-, mono(trifluoroacetate) (9CI)
 MF C34 H36 Cl2 N6 O6 S . C2 H F3 O2

CM 1

Absolute stereochemistry.

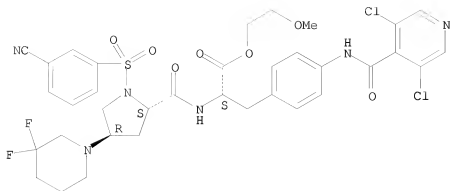


CM 2



L3 102 ANSWERS REGISTRY COPYRIGHT 2008 ACS on STN
 IN L-Phenylalanine, (4R)-1-[(3-cyanophenyl)sulfonyl]-4-(3,3-difluoro-1-piperidinyl)-L-prolyl-4-[[[(3,5-dichloro-4-pyridinyl)carbonyl]amino]-, 2-methoxyethyl ester (9CI)
 MF C35 H36 Cl2 F2 N6 O7 S

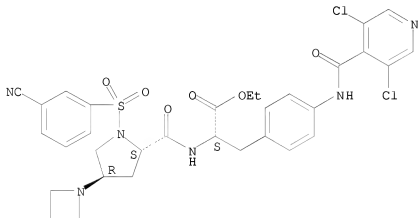
Absolute stereochemistry.



PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

L3 102 ANSWERS REGISTRY COPYRIGHT 2008 ACS on STN
 IN L-Phenylalanyl, (4R)-4-(1-azetidinyl)-1-[(3-cyanophenyl)sulfonyl]-L-
 prolyl-4-[[[(3,5-dichloro-4-pyridinyl)carbonyl]amino]-, ethyl ester (9CI)
 MF C32 H32 Cl2 N6 O6 S

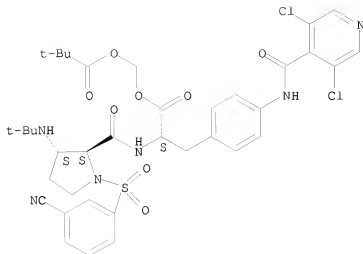
Absolute stereochemistry.



PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

L3 102 ANSWERS REGISTRY COPYRIGHT 2008 ACS on STN
 IN L-Phenylalanyl, (3S)-1-[(3-cyanophenyl)sulfonyl]-3-[(1,1-
 dimethylethyl)amino]-L-prolyl-4-[[[(3,5-dichloro-4-
 pyridinyl)carbonyl]amino]-, (2,2-dimethyl-1-oxopropoxy)methyl ester (9CI)
 MF C37 H42 Cl2 N6 O8 S

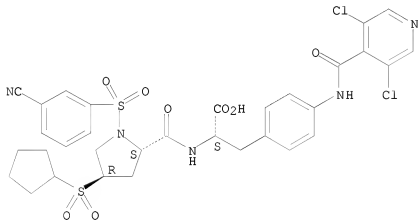
Absolute stereochemistry.



PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

L3 102 ANSWERS REGISTRY COPYRIGHT 2008 ACS on STN
 IN L-Phenylalanine, (4R)-1-[(3-cyanophenyl)sulfonyl]-4-(cyclopentylsulfonyl)-
 L-prolyl-4-[[[(3,5-dichloro-4-pyridinyl)carbonyl]amino]- (9CI)
 MF C32 H31 Cl2 N5 O8 S2

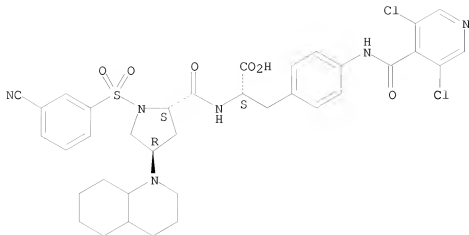
Absolute stereochemistry.



PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

L3 102 ANSWERS REGISTRY COPYRIGHT 2008 ACS on STN
 IN L-Phenylalanine, (4R)-1-[(3-cyanophenyl)sulfonyl]-4-(octahydro-1(2H)-
 quinoliny)-L-prolyl-4-[[[(3,5-dichloro-4-pyridinyl)carbonyl]amino]- (9CI)
 MF C36 H38 Cl2 N6 O6 S
 CI COM

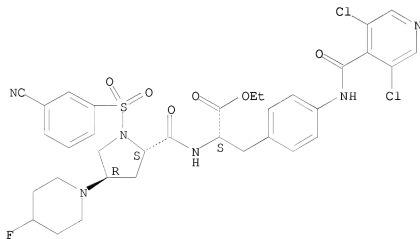
Absolute stereochemistry.



PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

L3 102 ANSWERS REGISTRY COPYRIGHT 2008 ACS on STN
 IN L-Phenylalanine, (4R)-1-[(3-cyanophenyl)sulfonyl]-4-(4-fluoro-1-piperidinyl)-L-prolyl-4-[[3,5-dichloro-4-pyridinyl]carbonylamino]-ethyl ester (9CI)
 MF C34 H35 Cl2 F N6 O6 S

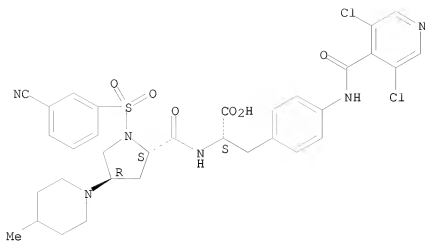
Absolute stereochemistry.



PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

L3 102 ANSWERS REGISTRY COPYRIGHT 2008 ACS on STN
 IN L-Phenylalanine, (4R)-1-[(3-cyanophenyl)sulfonyl]-4-(4-methyl-1-piperidinyl)-L-prolyl-4-[[3,5-dichloro-4-pyridinyl]carbonylamino]-ethyl ester (9CI)
 MF C33 H34 Cl2 N6 O6 S
 CI COM

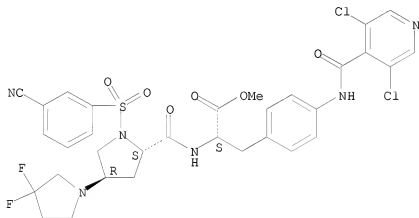
Absolute stereochemistry.



PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

L3 102 ANSWERS REGISTRY COPYRIGHT 2008 ACS on STN
 IN L-Phenylalanine, (4R)-1-[(3-cyanophenyl)sulfonyl]-4-(3,3-difluoro-1-pyrrolidinyl)-L-prolyl-4-[[(3,5-dichloro-4-pyridinyl)carbonyl]amino]-, methyl ester (9CI)
 MF C32 H30 Cl2 F2 N6 O6 S

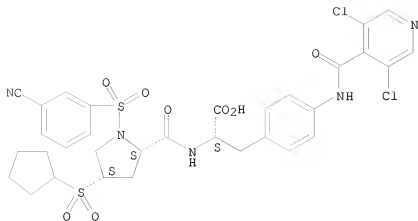
Absolute stereochemistry.



PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

L3 102 ANSWERS REGISTRY COPYRIGHT 2008 ACS on STN
 IN L-Phenylalanine, (4S)-1-[(3-cyanophenyl)sulfonyl]-4-(cyclopentylsulfonyl)-L-prolyl-4-[[(3,5-dichloro-4-pyridinyl)carbonyl]amino]- (9CI)
 MF C32 H31 Cl2 N5 O8 S2

Absolute stereochemistry.

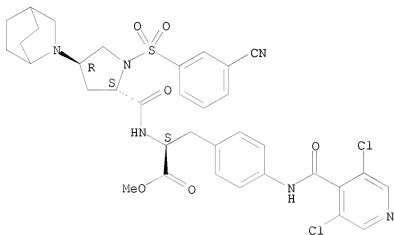


PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

L3 102 ANSWERS REGISTRY COPYRIGHT 2008 ACS on STN
 IN L-Phenylalanine, (4R)-4-(2-azabicyclo[2.2.2]oct-2-yl)-1-[(3-cyanophenyl)sulfonyl]-L-prolyl-4-[[[(3,5-dichloro-4-pyridinyl)carbonyl]amino]-, methyl ester, mono(trifluoroacetate) (9CI)
 MF C35 H36 Cl2 N6 O6 S . C2 H F3 O2

CM 1

Absolute stereochemistry.

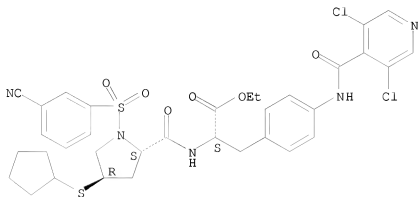


CM 2



L3 102 ANSWERS REGISTRY COPYRIGHT 2008 ACS on STN
 IN L-Phenylalanine, (4R)-1-[(3-cyanophenyl)sulfonyl]-4-(cyclopentylthio)-L-
 prolyl-4-[[[(3,5-dichloro-4-pyridinyl)carbonyl]amino]-, ethyl ester (9CI)
 MF C34 H35 Cl2 N5 O6 S2

Absolute stereochemistry.

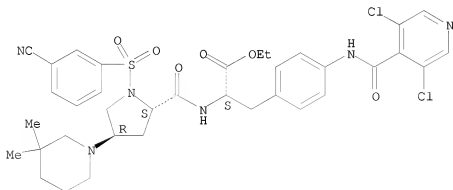


PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

L3 102 ANSWERS REGISTRY COPYRIGHT 2008 ACS on STN
 IN L-Phenylalanine, (4R)-1-[(3-cyanophenyl)sulfonyl]-4-(3,3-dimethyl-1-
 piperidinyl)-L-prolyl-4-[[[(3,5-dichloro-4-pyridinyl)carbonyl]amino]-,
 ethyl ester, mono(trifluoroacetate) (9CI)
 MF C36 H40 Cl2 N6 O6 S . C2 H F3 O2

CM 1

Absolute stereochemistry.

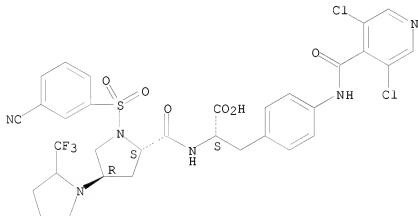


CM 2



L3 102 ANSWERS REGISTRY COPYRIGHT 2008 ACS on STN
 IN L-Phenylalanine, (4R)-1-[(3-cyanophenyl)sulfonyl]-4-[2-(trifluoromethyl)-1-pyrrolidiny]-L-prolyl-4-[[3,5-dichloro-4-pyridinyl)carbonyl]amino]-(9CI)
 MF C32 H29 Cl2 F3 N6 O6 S

Absolute stereochemistry.

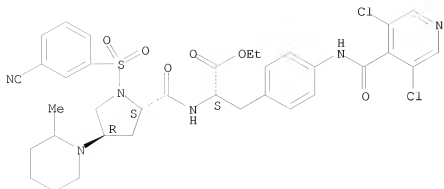


PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

L3 102 ANSWERS REGISTRY COPYRIGHT 2008 ACS on STN
 IN L-Phenylalanine, (4R)-1-[(3-cyanophenyl)sulfonyl]-4-(2-methyl-1-piperidiny)-L-prolyl-4-[[3,5-dichloro-4-pyridinyl)carbonyl]amino]-ethyl ester, mono(trifluoroacetate) (9CI)
 MF C35 H38 Cl2 N6 O6 S . C2 H F3 O2

CM 1

Absolute stereochemistry.

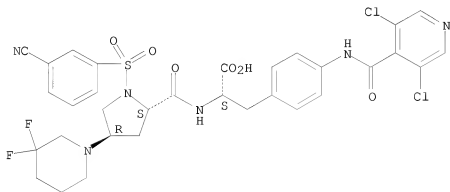


CM 2



L3 102 ANSWERS REGISTRY COPYRIGHT 2008 ACS on STN
 IN L-Phenylalanine, (4R)-1-[(3-cyanophenyl)sulfonyl]-4-[(3,3-difluoro-1-
 piperidinyl)-L-prolyl-4-[[[(3,5-dichloro-4-pyridinyl)carbonyl]amino]- (9CI)
 MF C32 H30 Cl2 F2 N6 O6 S

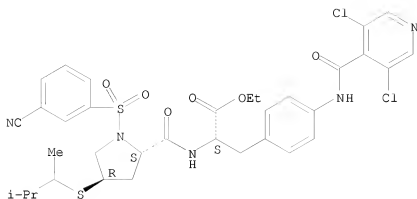
Absolute stereochemistry.



PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

L3 102 ANSWERS REGISTRY COPYRIGHT 2008 ACS on STN
 IN L-Phenylalanine, (4R)-1-[(3-cyanophenyl)sulfonyl]-4-[(1,2-
 dimethylpropyl)thio]-L-prolyl-4-[[[(3,5-dichloro-4-
 pyridinyl)carbonyl]amino]-, ethyl ester (9CI)
 MF C34 H37 Cl2 N5 O6 S2

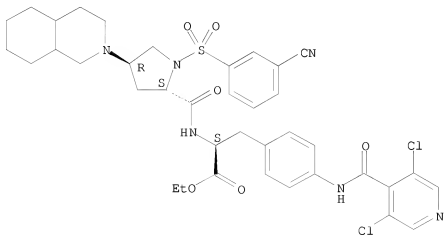
Absolute stereochemistry.



PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

L3 102 ANSWERS REGISTRY COPYRIGHT 2008 ACS on STN
 IN L-Phenylalanine, (4R)-1-[(3-cyanophenyl)sulfonyl]-4-(octahydro-2(1H)-
 isoquinolinyl)-L-prolyl-4-[[(3,5-dichloro-4-pyridinyl)carbonyl]amino]-,
 ethyl ester (9CI)
 MF C38 H42 Cl2 N6 O6 S
 CI COM

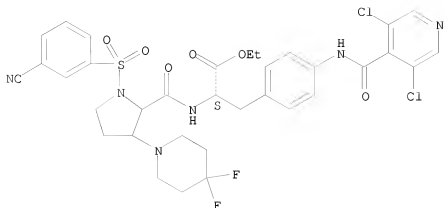
Absolute stereochemistry.



PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

L3 102 ANSWERS REGISTRY COPYRIGHT 2008 ACS on STN
 IN L-Phenylalanine, 1-[(3-cyanophenyl)sulfonyl]-3-(4,4-difluoro-1-
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 ester (9CI)
 MF C34 H34 Cl2 F2 N6 O6 S

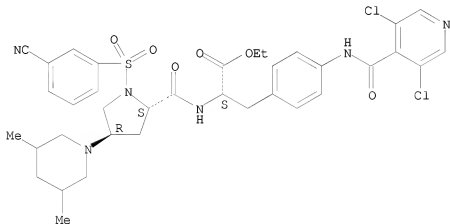
Absolute stereochemistry.



PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

L3 102 ANSWERS REGISTRY COPYRIGHT 2008 ACS on STN
 IN L-Phenylalanine, (4R)-1-[(3-cyanophenyl)sulfonyl]-4-(3,5-dimethyl-1-piperidinyl)-L-prolyl-4-[[(3,5-dichloro-4-pyridinyl)carbonyl]amino]-, ethyl ester (9CI)
 MF C36 H40 Cl2 N6 O6 S
 CI COM

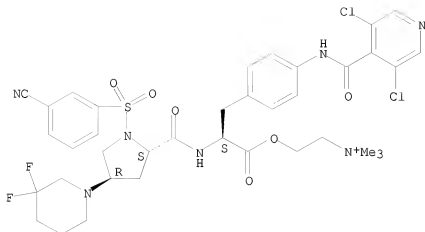
Absolute stereochemistry.



PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

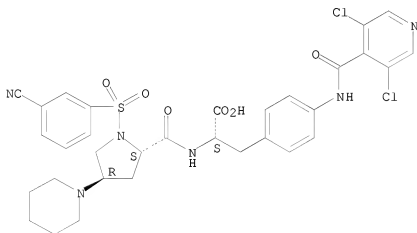
L3 102 ANSWERS REGISTRY COPYRIGHT 2008 ACS on STN
 IN L-Phenylalanine, (4R)-1-[(3-cyanophenyl)sulfonyl]-4-(3,3-difluoro-1-piperidinyl)-L-prolyl-4-[[(3,5-dichloro-4-pyridinyl)carbonyl]amino]-, 2-(trimethylammonio)ethyl ester (9CI)
 MF C37 H42 Cl2 F2 N7 O6 S

Absolute stereochemistry.



L3 102 ANSWERS REGISTRY COPYRIGHT 2008 ACS on STN
 IN L-Phenylalanine, (4R)-1-[(3-cyanophenyl)sulfonyl]-4-[(1-piperidinyl)-L-prolyl-4-[(3,5-dichloro-4-pyridinyl)carbonyl]amino]- (9CI)
 MF C32 H32 Cl2 N6 O6 S
 CI COM

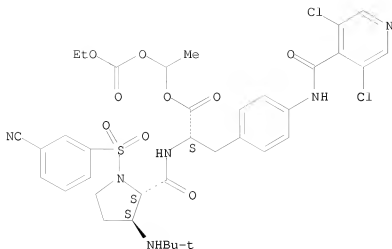
Absolute stereochemistry.



PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

L3 102 ANSWERS REGISTRY COPYRIGHT 2008 ACS on STN
 IN L-Phenylalanine, (3S)-1-[(3-cyanophenyl)sulfonyl]-3-[(1,1-dimethylethyl)amino]-L-prolyl-4-[(3,5-dichloro-4-pyridinyl)carbonyl]amino]-, 1-[(ethoxycarbonyl)oxy]ethyl ester (9CI)
 MF C36 H40 Cl2 N6 O9 S

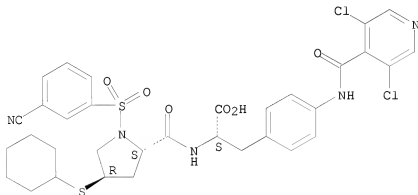
Absolute stereochemistry.



PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

L3 102 ANSWERS REGISTRY COPYRIGHT 2008 ACS on STN
 IN L-Phenylalanine, (4R)-1-[(3-cyanophenyl)sulfonyl]-4-(cyclohexylthio)-L-
 prolyl-4-[[(3,5-dichloro-4-pyridinyl)carbonyl]amino]- (9CI)
 MF C33 H33 Cl2 N5 O6 S2

Absolute stereochemistry.

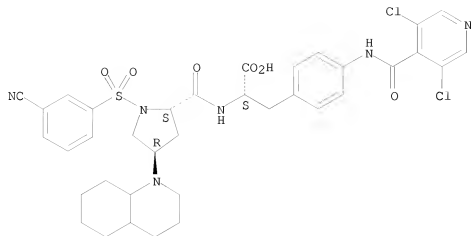


PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

L3 102 ANSWERS REGISTRY COPYRIGHT 2008 ACS on STN
 IN L-Phenylalanine, (4R)-1-[(3-cyanophenyl)sulfonyl]-4-(octahydro-1(2H)-
 quinolinyL)-L-prolyl-4-[[(3,5-dichloro-4-pyridinyl)carbonyl]amino]-,
 mono(trifluoroacetate) (9CI)
 MF C36 H38 Cl2 N6 O6 S . C2 H F3 O2

CM 1

Absolute stereochemistry.

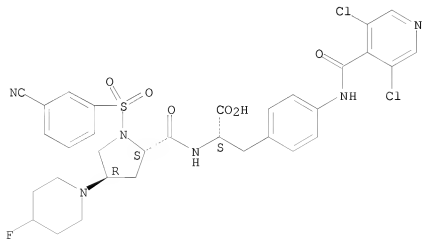


CM 2



L3 102 ANSWERS REGISTRY COPYRIGHT 2008 ACS on STN
 IN L-Phenylalanine, (4R)-1-[(3-cyanophenyl)sulfonyl]-4-(4-fluoro-1-
 piperidinyl)-L-prolyl-4-[[[(3,5-dichloro-4-pyridinyl)carbonylamino]- (9CI)
 MF C32 H31 Cl2 F N6 O6 S

Absolute stereochemistry.

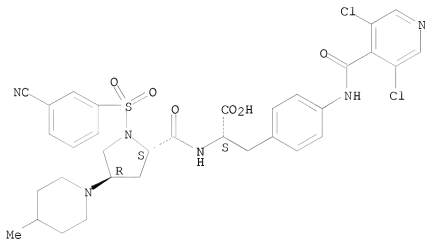


PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

L3 102 ANSWERS REGISTRY COPYRIGHT 2008 ACS on STN
 IN L-Phenylalanine, (4R)-1-[(3-cyanophenyl)sulfonyl]-4-(4-methyl-1-piperidinyl)-L-prolyl-4-[[[(3,5-dichloro-4-pyridinyl)carbonyl]amino]-, mono(trifluoroacetate) (9CI)
 MF C33 H34 Cl2 N6 O6 S . C2 H F3 O2

CM 1

Absolute stereochemistry.

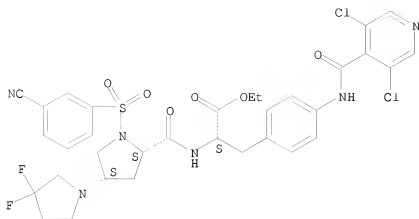


CM 2



L3 102 ANSWERS REGISTRY COPYRIGHT 2008 ACS on STN
 IN L-Phenylalanine, (4S)-1-[(3-cyanophenyl)sulfonyl]-4-(3,3-difluoro-1-pyrrolidinyl)-L-prolyl-4-[[[(3,5-dichloro-4-pyridinyl)carbonyl]amino]-, ethyl ester (9CI)
 MF C33 H32 Cl2 F2 N6 O6 S

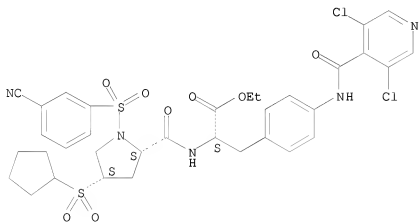
Absolute stereochemistry.



PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

L3 102 ANSWERS REGISTRY COPYRIGHT 2008 ACS on STN
 IN L-Phenylalanine, (4S)-1-[(3-cyanophenyl)sulfonyl]-4-(cyclopentylsulfonyl)-
 L-prolyl-4-[[[(3,5-dichloro-4-pyridinyl)carbonylamino]-, ethyl ester (9CI)
 MF C34 H35 Cl2 N5 O8 S2

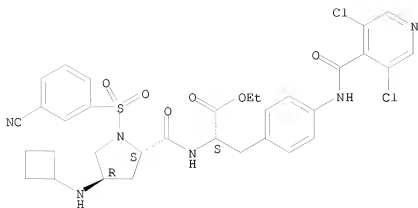
Absolute stereochemistry.



PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

L3 102 ANSWERS REGISTRY COPYRIGHT 2008 ACS on STN
 IN L-Phenylalanine, (4R)-1-[(3-cyanophenyl)sulfonyl]-4-(cyclobutylamino)-L-
 prolyl-4-[[[(3,5-dichloro-4-pyridinyl)carbonylamino]-, ethyl ester (9CI)
 MF C33 H34 Cl2 N6 O6 S
 CI COM

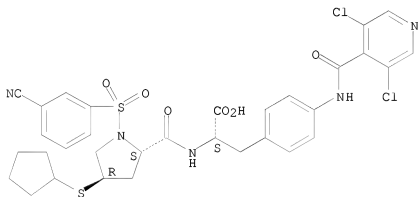
Absolute stereochemistry.



PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

L3 102 ANSWERS REGISTRY COPYRIGHT 2008 ACS on STN
 IN L-Phenylalanine, (4R)-1-[(3-cyanophenyl)sulfonyl]-4-(cyclopentylthio)-L-prolyl-4-[[[(3,5-dichloro-4-pyridinyl)carbonyl]amino]- (9CI)
 MF C32 H31 Cl2 N5 O6 S2

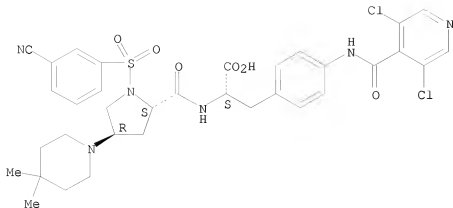
Absolute stereochemistry.



PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

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 MF C34 H36 Cl2 N6 O6 S
 CI COM

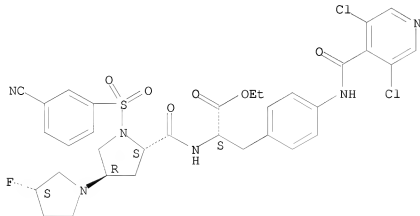
Absolute stereochemistry.



PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

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 IN L-Phenylalanine, (4R)-1-[(3-cyanophenyl)sulfonyl]-4-[(3S)-3-fluoro-1-pyrrolidinyl]-L-prolyl-4-[[[(3,5-dichloro-4-pyridinyl)carbonyl]amino]-ethyl ester (9CI)
 MF C33 H33 Cl2 F N6 O6 S

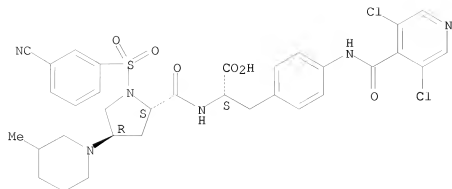
Absolute stereochemistry.



PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

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 MF C33 H34 Cl2 N6 O6 S
 CI COM

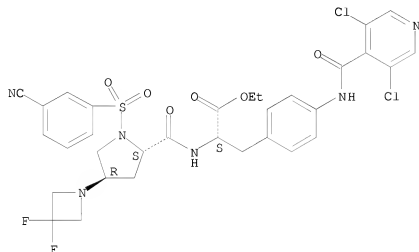
Absolute stereochemistry.



PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

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 MF C32 H30 Cl2 F2 N6 O6 S

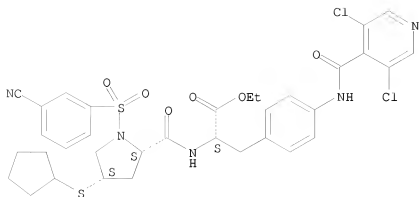
Absolute stereochemistry.



PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

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 IN L-Phenylalanine, (4S)-1-[(3-cyanophenyl)sulfonyl]-4-(cyclopentylthio)-L-prolyl-4-[[[(3,5-dichloro-4-pyridinyl)carbonylamino]-, ethyl ester (9CI)
 MF C34 H35 Cl2 N5 O6 S2

Absolute stereochemistry.

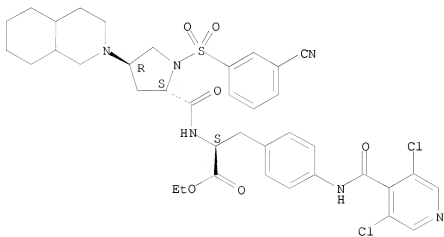


PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

L3 102 ANSWERS REGISTRY COPYRIGHT 2008 ACS on STN
 IN L-Phenylalanine, (4R)-1-[(3-cyanophenyl)sulfonyl]-4-(octahydro-2(1H)-
 isoquinolinyl)-L-prolyl-4-[[[(3,5-dichloro-4-pyridinyl)carbonyl]amino]-
 ethyl ester, mono(trifluoroacetate) (9CI)
 MF C38 H42 Cl2 N6 O6 S . C2 H F3 O2

CM 1

Absolute stereochemistry.



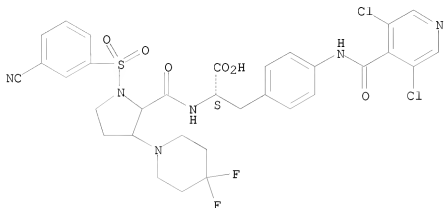
CM 2



L3 102 ANSWERS REGISTRY COPYRIGHT 2008 ACS on STN

IN L-Phenylalanine, 1-[(3-cyanophenyl)sulfonyl]-3-(4,4-difluoro-1-piperidinyl)prolyl-4-[[[(3,5-dichloro-4-pyridinyl)carbonyl]amino]- (9CI)
 MF C32 H30 Cl2 F2 N6 O6 S

Absolute stereochemistry.

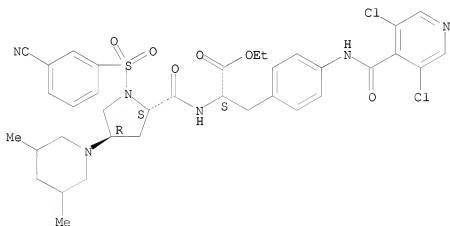


PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

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 IN L-Phenylalanine, (4R)-1-[(3-cyanophenyl)sulfonyl]-4-(3,5-dimethyl-1-piperidinyl)-L-prolyl-4-[[[(3,5-dichloro-4-pyridinyl)carbonyl]amino]-, ethyl ester, mono(trifluoroacetate) (9CI)
 MF C36 H40 Cl2 N6 O6 S . C2 H F3 O2

CM 1

Absolute stereochemistry.

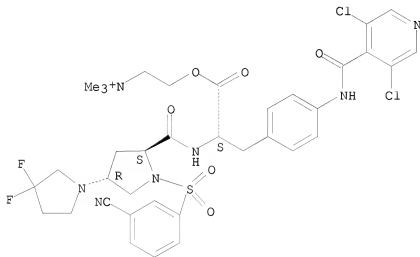


CM 2



L3 102 ANSWERS REGISTRY COPYRIGHT 2008 ACS on STN
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 MF C36 H40 Cl2 F2 N7 O6 S

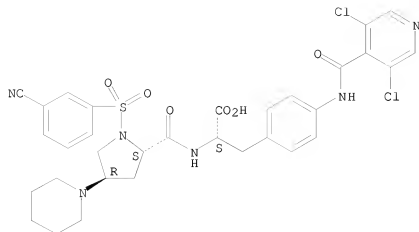
Absolute stereochemistry.



L3 102 ANSWERS REGISTRY COPYRIGHT 2008 ACS on STN
 IN L-Phenylalanine, (4R)-1-[(3-cyanophenyl)sulfonyl]-4-(1-piperidiny)-L-prolyl-4-[[[(3,5-dichloro-4-pyridinyl)carbonyl]amino]-, mono(trifluoroacetate) (9CI)
 MF C32 H32 Cl2 N6 O6 S . C2 H F3 O2

CM 1

Absolute stereochemistry.

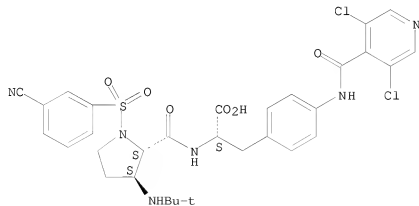


CM 2



L3 102 ANSWERS REGISTRY COPYRIGHT 2008 ACS on STN
 IN L-Phenylalanine, (3S)-1-[(3-cyanophenyl)sulfonyl]-3-[(1,1-
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 pyridinyl)carbonylamino]-, monosodium salt (9CI)
 MF C31 H32 Cl2 N6 O6 S . Na

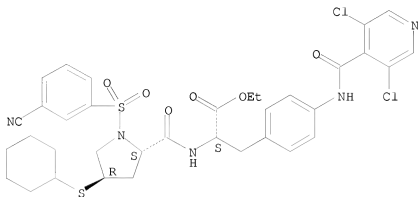
Absolute stereochemistry.



● Na

L3 102 ANSWERS REGISTRY COPYRIGHT 2008 ACS on STN
 IN L-Phenylalanine, (4R)-1-[(3-cyanophenyl)sulfonyl]-4-(cyclohexylthio)-L-
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 MF C35 H37 Cl2 N5 O6 S2

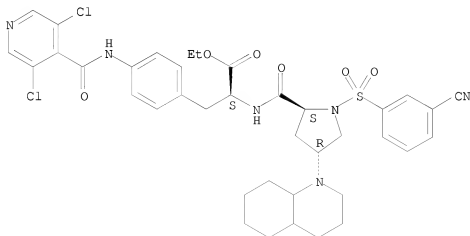
Absolute stereochemistry.



PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

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 IN L-Phenylalanine, (4R)-1-[(3-cyanophenyl)sulfonyl]-4-(octahydro-1(2H)-
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 ester (9CI)
 MF C38 H42 Cl2 N6 O6 S
 CI COM

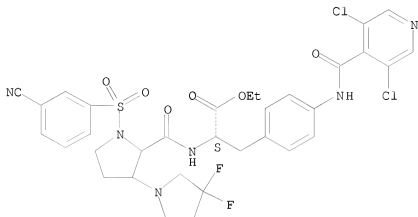
Absolute stereochemistry.



PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

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 MF C33 H32 Cl2 F2 N6 O6 S

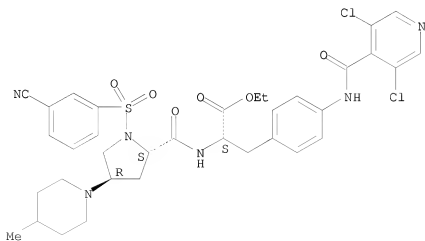
Absolute stereochemistry.



PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

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 IN L-Phenylalanine, (4R)-1-[(3-cyanophenyl)sulfonyl]-4-(4-methyl-1-piperidinyl)-L-prolyl-4-[[[(3,5-dichloro-4-pyridinyl)carbonyl]amino]-ethyl ester (9CI)
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 CI COM

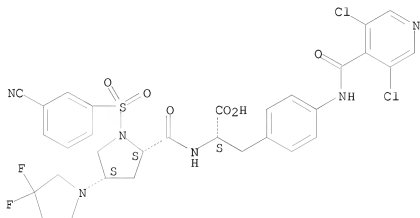
Absolute stereochemistry.



PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

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 IN L-Phenylalanine, (4S)-1-[(3-cyanophenyl)sulfonyl]-4-(3,3-difluoro-1-pyrrolidinyl)-L-prolyl-4-[[[(3,5-dichloro-4-pyridinyl)carbonyl]amino]-
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 MF C31 H28 Cl2 F2 N6 O6 S

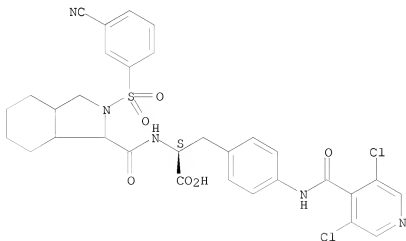
Absolute stereochemistry.



PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

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 MF C31 H29 Cl2 N5 O6 S

Absolute stereochemistry.

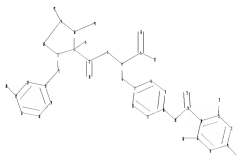
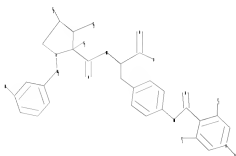


PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

ALL ANSWERS HAVE BEEN SCANNED

=>

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ring nodes :
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36
chain bonds :
1-2 1-45 2-3 2-25 3-4 4-5 4-6 5-26 5-27 6-7 10-28 13-17 15-42 16-43
17-18 22-24 28-29 29-30 29-31 32-37 34-47 36-38
ring bonds :
1-13 1-16 7-8 7-12 8-9 9-10 10-11 11-12 13-14 14-15 15-16 18-19 18-23
19-20 20-21 21-22 22-23 30-32 30-36 32-33 33-34 34-35 35-36
exact/norm bonds :
1-13 1-16 1-45 2-3 2-25 3-4 5-26 5-27 10-28 13-14 13-17 14-15 15-16
15-42 16-43 28-29 29-31 32-37 34-47 36-38
exact bonds :
1-2 4-5 4-6 6-7 17-18 22-24 29-30
normalized bonds :
7-8 7-12 8-9 9-10 10-11 11-12 18-19 18-23 19-20 20-21 21-22 22-23 30-32
30-36 32-33 33-34 34-35 35-36

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G1:X, MeO, EtO, n-PrO, i-PrO, CH₃, CH₂, CH, Et, n-Pr, i-Pr

G2:H, N

G3:H,CH3

Match level :

1:Atom 2:CLASS 3:CLASS 4:CLASS 5:CLASS 6:CLASS 7:Atom 8:Atom 9:Atom
10:Atom 11:Atom 12:Atom 13:Atom 14:Atom 15:Atom 16:Atom 17:CLASS 18:Atom
19:Atom 20:Atom 21:Atom 22:Atom 23:Atom 24:CLASS 25:CLASS 26:CLASS 27:CLASS
28:CLASS 29:CLASS 30:Atom 31:CLASS 32:Atom 33:Atom 34:Atom 35:Atom 36:Atom
37:CLASS 38:CLASS 42:CLASS 43:CLASS 45:CLASS 47:CLASS

L10 STRUCTURE UPLOADED

=> s l10 sam

SAMPLE SEARCH INITIATED 18:23:53 FILE 'REGISTRY'

SAMPLE SCREEN SEARCH COMPLETED - 0 TO ITERATE

100.0% PROCESSED 0 ITERATIONS

0 ANSWERS

SEARCH TIME: 00.00.01

FULL FILE PROJECTIONS: ONLINE **COMPLETE**

BATCH **COMPLETE**

PROJECTED ITERATIONS: 0 TO 0

PROJECTED ANSWERS: 0 TO 0

L11 0 SEA SSS SAM L10

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FULL SEARCH INITIATED 18:23:58 FILE 'REGISTRY'

FULL SCREEN SEARCH COMPLETED - 0 TO ITERATE

100.0% PROCESSED 0 ITERATIONS

0 ANSWERS

SEARCH TIME: 00.00.01

L12 0 SEA SSS FUL L10

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(FILE 'HOME' ENTERED AT 18:12:29 ON 11 NOV 2008)

FILE 'REGISTRY' ENTERED AT 18:12:36 ON 11 NOV 2008

L1 STRUCTURE UPLOADED

L2 10 S L1 SAM

L3 102 S L1 FULL

FILE 'STNGUIDE' ENTERED AT 18:13:28 ON 11 NOV 2008

FILE 'REGISTRY' ENTERED AT 18:14:27 ON 11 NOV 2008

L4 STRUCTURE UPLOADED

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L6 0 S L4 FULL SUB=L3

FILE 'CAPLUS' ENTERED AT 18:18:15 ON 11 NOV 2008

L7 4 S L3

L8 1 S US20070179190/PN

FILE 'MEDLINE, BIOSIS, EMBASE' ENTERED AT 18:19:51 ON 11 NOV 2008

L9 0 S L3

FILE 'STNGUIDE' ENTERED AT 18:20:04 ON 11 NOV 2008

FILE 'REGISTRY' ENTERED AT 18:21:49 ON 11 NOV 2008
L10 STRUCTURE UPLOADED
L11 0 S L10 SAM
L12 0 S L10 FULL

=> log h

COST IN U.S. DOLLARS	SINCE FILE ENTRY	TOTAL SESSION
FULL ESTIMATED COST	179.74	423.36
DISCOUNT AMOUNTS (FOR QUALIFYING ACCOUNTS)	SINCE FILE ENTRY	TOTAL SESSION
CA SUBSCRIBER PRICE	0.00	-0.80

SESSION WILL BE HELD FOR 120 MINUTES
STN INTERNATIONAL SESSION SUSPENDED AT 18:24:06 ON 11 NOV 2008
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PASSWORD:

* * * * * RECONNECTED TO STN INTERNATIONAL * * * * *
SESSION RESUMED IN FILE 'REGISTRY' AT 18:39:30 ON 11 NOV 2008
FILE 'REGISTRY' ENTERED AT 18:39:30 ON 11 NOV 2008
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COST IN U.S. DOLLARS	SINCE FILE ENTRY	TOTAL SESSION
FULL ESTIMATED COST	179.74	423.36
DISCOUNT AMOUNTS (FOR QUALIFYING ACCOUNTS)	SINCE FILE ENTRY	TOTAL SESSION
CA SUBSCRIBER PRICE	0.00	-0.80

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(FILE 'HOME' ENTERED AT 18:12:29 ON 11 NOV 2008)

FILE 'REGISTRY' ENTERED AT 18:12:36 ON 11 NOV 2008
L1 STRUCTURE UPLOADED
L2 10 S L1 SAM
L3 102 S L1 FULL

FILE 'STNGUIDE' ENTERED AT 18:13:28 ON 11 NOV 2008

FILE 'REGISTRY' ENTERED AT 18:14:27 ON 11 NOV 2008
L4 STRUCTURE UPLOADED
L5 0 S L4 SAM SUB=L3
L6 0 S L4 FULL SUB=L3

FILE 'CAPLUS' ENTERED AT 18:18:15 ON 11 NOV 2008
L7 4 S L3
L8 1 S US20070179190/PN

FILE 'MEDLINE, BIOSIS, EMBASE' ENTERED AT 18:19:51 ON 11 NOV 2008

L9

0 S L3

FILE 'STNGUIDE' ENTERED AT 18:20:04 ON 11 NOV 2008

FILE 'REGISTRY' ENTERED AT 18:21:49 ON 11 NOV 2008

L10 STRUCTURE UPLOADED

L11 0 S L10 SAM

L12 0 S L10 FULL

=> fil caplus

COST IN U.S. DOLLARS

SINCE FILE

TOTAL

ENTRY

SESSION

FULL ESTIMATED COST

179.74

423.36

DISCOUNT AMOUNTS (FOR QUALIFYING ACCOUNTS)

SINCE FILE

TOTAL

ENTRY

SESSION

CA SUBSCRIBER PRICE

0.00

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FILE 'CAPLUS' ENTERED AT 18:39:45 ON 11 NOV 2008

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FILE COVERS 1907 - 11 Nov 2008 VOL 149 ISS 20

FILE LAST UPDATED: 10 Nov 2008 (20081110/ED)

Caplus now includes complete International Patent Classification (IPC) reclassification data for the second quarter of 2008.

Effective October 17, 2005, revised CAS Information Use Policies apply. They are available for your review at:

<http://www.cas.org/legal/infopolicy.html>

'OBI' IS DEFAULT SEARCH FIELD FOR 'CAPLUS' FILE

=> d ti l7 1-4

L7 ANSWER 1 OF 4 CAPLUS COPYRIGHT 2008 ACS on STN

TI Preparation of prolyl peptide derivatives as VLA-4 antagonists

L7 ANSWER 2 OF 4 CAPLUS COPYRIGHT 2008 ACS on STN

TI Preparation of dipeptide derivatives as VLA-4 antagonists

L7 ANSWER 3 OF 4 CAPLUS COPYRIGHT 2008 ACS on STN

TI Preparation of prolylphenylalanine derivatives as VLA-4 antagonists

L7 ANSWER 4 OF 4 CAPLUS COPYRIGHT 2008 ACS on STN

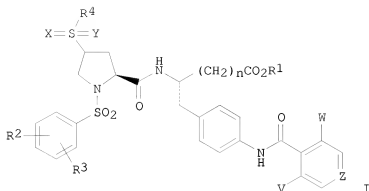
TI Preparation of N-arylsulfonyl aza-bicyclic derivatives as potent cell adhesion inhibitors

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 'IBIB ABS HITSTR ' IS NOT A VALID STRUCTURE FORMAT KEYWORD
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L7 ANSWER 1 OF 4 CAPLUS COPYRIGHT 2008 ACS on SIN
 ACCESSION NUMBER: 2006:1123323 CAPLUS
 DOCUMENT NUMBER: 145:455274
 TITLE: Preparation of prolyl peptide derivatives as VLA-4 antagonists
 INVENTOR(S): Stock, Nicholas S.; Smith, Nicholas D.; Munoz, Benito
 PATENT ASSIGNEE(S): Merck & Co., Inc., USA
 SOURCE: PCT Int. Appl., 29pp.
 CODEN: PIXXD2
 DOCUMENT TYPE: Patent
 LANGUAGE: English
 FAMILY ACC. NUM. COUNT: 1
 PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
WO 2006113199	A1	20061026	WO 2006-US13254	20060410
W: AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BW, BY, BZ, CA, CH, CN, CO, CR, CU, CZ, DE, DK, DM, DZ, EC, EE, EG, ES, FI, GB, GD, GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KM, KN, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, LY, MA, MD, MG, MK, MN, MW, MX, MZ, NA, NG, NI, NO, NZ, OM, PG, PH, PL, PT, RO, RU, SC, SD, SE, SG, SK, SL, SM, SY, TJ, TM, TN, TR, TT, TZ, UA, UG, US, UZ, VC, VN, YU, ZA, ZM, ZW				
RM: AT, BE, BG, CH, CY, CZ, DE, DK, EE, ES, FI, FR, GB, GR, HU, IE, IS, IT, LT, LU, LV, MC, NL, PL, PT, RO, SE, SI, SK, TR, BF, BJ, CF, CG, CI, CM, GA, GN, GQ, GW, ML, MR, NE, SN, TD, TG, BW, GH, GM, KE, LS, MW, MZ, NA, SD, SL, SZ, TZ, UG, ZM, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM				
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JP 2008536850	T	20080911	JP 2008-506564	20060410
IN 2007CN04219	A	20071221	IN 2007-CN4219	20070924
CN 101155798	A	20080402	CN 2006-80011232	20071008
PRIORITY APPLN. INFO.:			US 2005-671352P	P 20050414
			WO 2006-US13254	W 20060410
OTHER SOURCE(S):		MARPAT 145:455274		
GI				



AB The invention relates to 4(R or S)-thio-, -sulfenyl and -sulfonyl proline derivs. I [n is 0 or 1; V, W are independently alkyl, halo, or alkoxy; X, Y are independently O or not present; Z is N or N:O; R1 is (un)substituted alkyl or aryl; R2, R3 are independently H, alkylsulfonyl, CN, CF3, OCF3, or halo; R4 is (un)substituted alkyl, alkenyl, alkynyl, or a cyclic group] or their pharmaceutically-acceptable salts, which are antagonists of the VLA-4 integrin and are useful in the treatment, prevention and suppression of diseases mediated by VLA-4-binding and cell adhesion and activation. Compds. of the invention demonstrate significant receptor occupancy of VLA-4 bearing cells after oral administration and are suitable for once-, twice-, or thrice-a-day oral administration. Thus, (4R)-prolyl peptide I (n = 0; V = W = Cl; X = Y = null; Z = N; R = Et; R2 = H; R3 = 3-CN; R4 = cyclopentyl) was prepared by sequential S-alkylation, peptide coupling, sulfonylation, and saponification

IT 913266-74-7P 913266-75-8P 913266-76-9P
 913266-77-0P 913266-78-1P 913266-79-2P
 913266-80-5P 913266-81-6P 913266-82-7P
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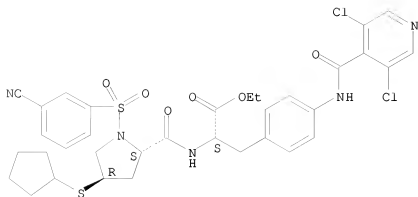
RL: PAC (Pharmacological activity); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)

(preparation of thio-, sulfenyl-, or sulfonyl-substituted prolyl peptide derivs. as VLA-4 antagonists)

RN 913266-74-7 CAPLUS

CN L-Phenylalanine, (4R)-1-[(3-cyanophenyl)sulfonyl]-4-(cyclopentylthio)-L-prolyl-4-[[[(3,5-dichloro-4-pyridinyl)carbonyl]amino]-, ethyl ester (9CI) (CA INDEX NAME)

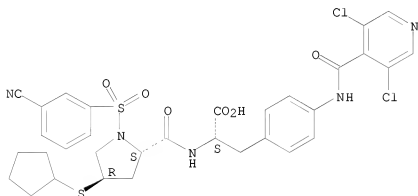
Absolute stereochemistry.



RN 913266-75-8 CAPLUS

CN L-Phenylalanine, (4R)-1-[(3-cyanophenyl)sulfonyl]-4-(cyclopentylthio)-L-prolyl-4-[[[(3,5-dichloro-4-pyridinyl)carbonyl]amino]- (9CI) (CA INDEX NAME)

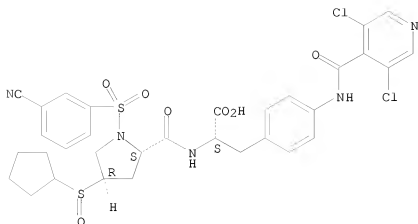
Absolute stereochemistry.



RN 913266-76-9 CAPLUS

CN L-Phenylalanine, (4R)-1-[(3-cyanophenyl)sulfonyl]-4-(cyclopentylsulfanyl)-L-prolyl-4-[[[(3,5-dichloro-4-pyridinyl)carbonyl]amino]- (9CI) (CA INDEX NAME)

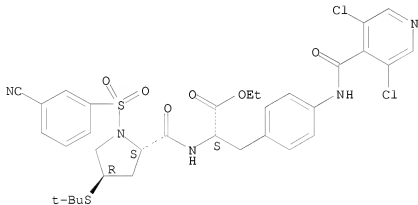
Absolute stereochemistry.



RN 913266-77-0 CAPLUS

CN L-Phenylalanine, (4R)-1-[(3-cyanophenyl)sulfonyl]-4-[(1,1-dimethylethylthio)-L-prolyl-4-[(3,5-dichloro-4-pyridinyl)carbonyl]amino]-, ethyl ester (9CI) (CA INDEX NAME)

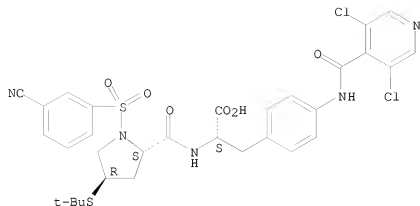
Absolute stereochemistry.



RN 913266-78-1 CAPLUS

CN L-Phenylalanine, (4R)-1-[(3-cyanophenyl)sulfonyl]-4-[(1,1-dimethylethylthio)-L-prolyl-4-[(3,5-dichloro-4-pyridinyl)carbonyl]amino]-, ethyl ester (9CI) (CA INDEX NAME)

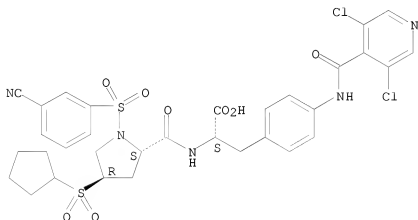
Absolute stereochemistry.



RN 913266-79-2 CAPLUS

CN L-Phenylalanine, (4R)-1-[(3-cyanophenyl)sulfonyl]-4-(cyclopentylsulfonyl)-
L-prolyl-4-[[[(3,5-dichloro-4-pyridinyl)carbonyl]amino]- (9CI) (CA INDEX
NAME)

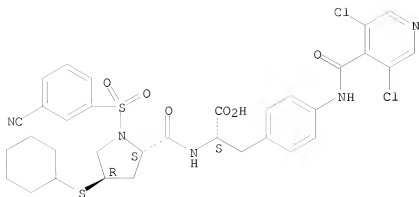
Absolute stereochemistry.



RN 913266-80-5 CAPLUS

CN L-Phenylalanine, (4R)-1-[(3-cyanophenyl)sulfonyl]-4-(cyclohexylthio)-L-
prolyl-4-[[[(3,5-dichloro-4-pyridinyl)carbonyl]amino]- (9CI) (CA INDEX
NAME)

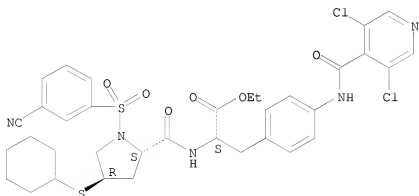
Absolute stereochemistry.



RN 913266-81-6 CAPLUS

CN L-Phenylalanine, (4R)-1-[(3-cyanophenyl)sulfonyl]-4-(cyclohexylthio)-L-prolyl-4-[[3,5-dichloro-4-pyridinyl)carbonyl]amino]-, ethyl ester (9CI) (CA INDEX NAME)

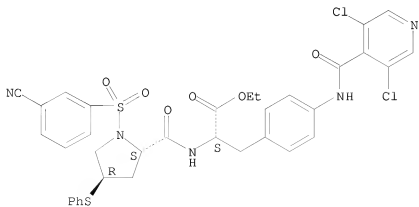
Absolute stereochemistry.



RN 913266-82-7 CAPLUS

CN L-Phenylalanine, (4R)-1-[(3-cyanophenyl)sulfonyl]-4-(phenylthio)-L-prolyl-4-[[3,5-dichloro-4-pyridinyl)carbonyl]amino]-, ethyl ester (9CI) (CA INDEX NAME)

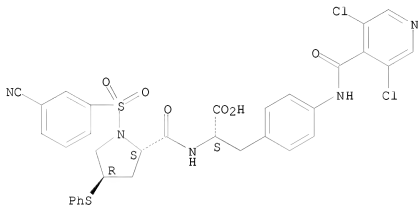
Absolute stereochemistry.



RN 913266-83-8 CAPLUS

CN L-Phenylalanine, (4R)-1-[(3-cyanophenyl)sulfonyl]-4-(phenylthio)-L-prolyl-4-[[[(3,5-dichloro-4-pyridinyl)carbonyl]amino]- (9CI) (CA INDEX NAME)

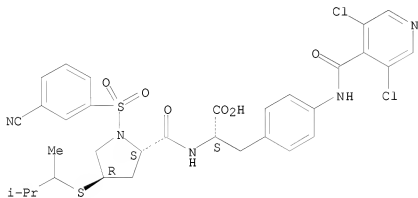
Absolute stereochemistry.



RN 913266-84-9 CAPLUS

CN L-Phenylalanine, (4R)-1-[(3-cyanophenyl)sulfonyl]-4-[(1,2-dimethylpropyl)thio]-L-prolyl-4-[[[(3,5-dichloro-4-pyridinyl)carbonyl]amino]- (9CI) (CA INDEX NAME)

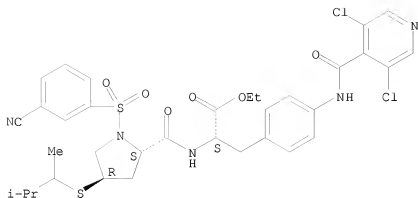
Absolute stereochemistry.



RN 913266-85-0 CAPLUS

CN L-Phenylalanine, (4R)-1-[(3-cyanophenyl)sulfonyl]-4-[(1,2-dimethylpropyl)thio]-L-prolyl-4-[[[(3,5-dichloro-4-pyridinyl)carbonyl]amino]-, ethyl ester (9CI) (CA INDEX NAME)

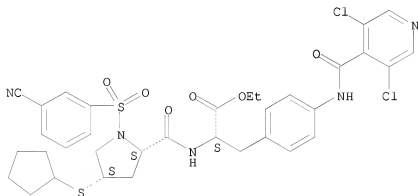
Absolute stereochemistry.



RN 913266-88-3 CAPLUS

L-Phenylalanine, (4S)-1-[(3-cyanophenyl)sulfonyl]-4-(cyclopentylthio)-L-
 prolyl-4-[[[(3,5-dichloro-4-pyridinyl)carbonyl]amino]-, ethyl ester (9CI)
 (CA INDEX NAME)

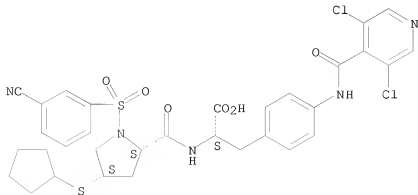
Absolute stereochemistry.



RN 913266-89-4 CAPLUS

CN L-Phenylalanine, (4S)-1-[(3-cyanophenyl)sulfonyl]-4-(cyclopentylthio)-L-propyl-4-[[[(3,5-dichloro-4-pyridinyl)carbonyl]amino]- (9CI) (CA INDEX NAME)

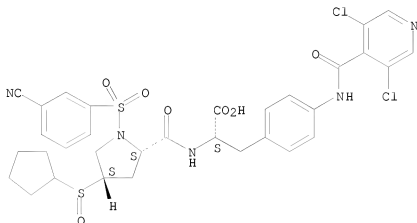
Absolute stereochemistry.



RN 913266-90-7 CAPLUS

CN L-Phenylalanine, (4S)-1-[(3-cyanophenyl)sulfonyl]-4-(cyclopentylsulfinyl)-
L-prolyl-4-[[(3,5-dichloro-4-pyridinyl)carbonylamino]- (9CI) (CA INDEX
NAME)

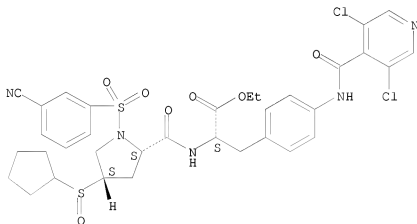
Absolute stereochemistry.



RN 913266-91-8 CAPLUS

CN L-Phenylalanine, (4S)-1-[(3-cyanophenyl)sulfonyl]-4-(cyclopentylsulfinyl)-
L-prolyl-4-[[(3,5-dichloro-4-pyridinyl)carbonylamino]-, ethyl ester (9CI)
(CA INDEX NAME)

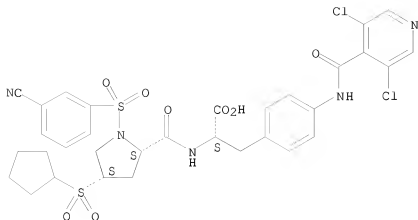
Absolute stereochemistry.



RN 913266-92-9 CAPLUS

CN L-Phenylalanine, (4S)-1-[(3-cyanophenyl)sulfonyl]-4-(cyclopentylsulfinyl)-
L-prolyl-4-[[(3,5-dichloro-4-pyridinyl)carbonylamino]- (9CI) (CA INDEX
NAME)

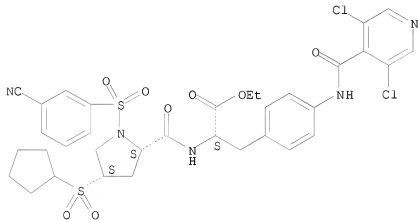
Absolute stereochemistry.



RN 913266-93-0 CAPLUS

CN L-Phenylalanine, (4S)-1-[(3-cyanophenyl)sulfonyl]-4-(cyclopentylsulfonyl)-L-prolyl-4-[[(3,5-dichloro-4-pyridinyl)carbonyl]amino]-, ethyl ester (9CI)
(CA INDEX NAME)

Absolute stereochemistry.



REFERENCE COUNT: 1 THERE ARE 1 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L7 ANSWER 2 OF 4 CAPLUS COPYRIGHT 2008 ACS on SIN

ACCESSION NUMBER: 2006:196055 CAPLUS

DOCUMENT NUMBER: 144:254393

TITLE: Preparation of dipeptide derivatives as VLA-4 antagonists

INVENTOR(S): Chen, Weichao; Lesback, Alec, D.; Munoz, Benito; Venkatraman, Shankar; Wang, Bowei

PATENT ASSIGNEE(S): Merck & Co., Inc., USA

SOURCE: PCI Int. Appl., 41 pp.

CODEN: PIXXD2

DOCUMENT TYPE: Patent

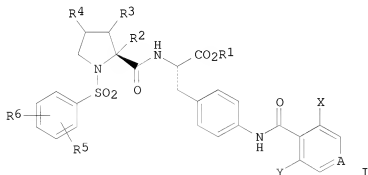
LANGUAGE: English

FAMILY ACC. NUM. COUNT: 1

PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
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WO 2006023396	A3	20060427		
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CN 101006097	A	20070725	CN 2005-80027718	20050812
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US 20070219252	A1	20070920	US 2007-659608	20070206
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PRIORITY APPLN. INFO.:			US 2004-601942P	P 20040816
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OTHER SOURCE(S):			CASREACT 144:254393; MARPAT 144:254393	
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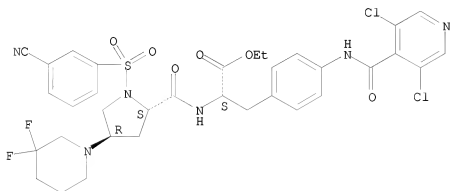


AB The invention relates to compds. I [A is N or N-0; X, Y are halo, alkyl or alkoxy; R1 is H or (un)substituted alkyl; R2 is H or Me; one of R3 and R4 is H and the other is 4-8 membered cyclic amine which is substituted by F, CF3, CO2H or ester; R5, R6 are independently H, alkylsulfonyl, CN, CF3, OCF3 or halo] or their pharmaceutically acceptable salts which are antagonists of VLA-4 and as such are useful in the inhibition or prevention of cell adhesion and cell-adhesion mediated pathologies such as inflammatory bowel disease. Thus, prolylphenylalanine derivative I (A = N; X, Y = Cl; R1 = Et; R2, R3, R5 = H; R4 = (R)-3,3-difluoropiperidino; R6 = 3-CN) was prepared by a multistep sequence involving reactions of 4-nitro-L-phenylalanine, 3,5-dichloroisonicotinic acid, cis-4-hydroxy-L-proline Me ester, 3-cyano-1-benzenesulfonyl chloride and 3,3-difluoropiperidine hydrochloride. Compds. of the invention demonstrated sustained and significant VLA-4 receptor occupancy (>50%)

after oral dosing.

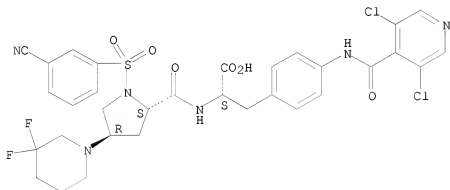
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RL: PAC (Pharmacological activity); RCT (Reactant); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); RACT (Reactant or reagent); USES (Uses)
(preparation of dipeptide derivs. as VLA-4 antagonists)
RN 877406-25-2 CAPLUS
CN L-Phenylalanine, (4R)-1-[(3-cyanophenyl)sulfonyl]-4-(3,3-difluoro-1-piperidinyl)-L-prolyl-4-[[[(3,5-dichloro-4-pyridinyl)carbonyl]amino]-ethyl ester (9CI) (CA INDEX NAME)

Absolute stereochemistry.



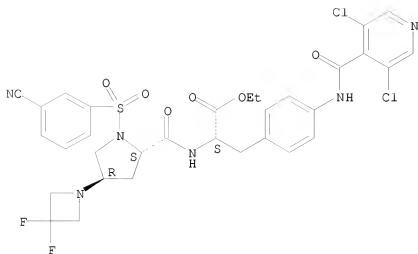
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(CA INDEX NAME)

Absolute stereochemistry.



RN 877406-27-4 CAPLUS
CN L-Phenylalanine, (4R)-1-[(3-cyanophenyl)sulfonyl]-4-(3,3-difluoro-1-azetidiny)-L-prolyl-4-[[[(3,5-dichloro-4-pyridinyl)carbonyl]amino]-, ethyl ester (9CI) (CA INDEX NAME)

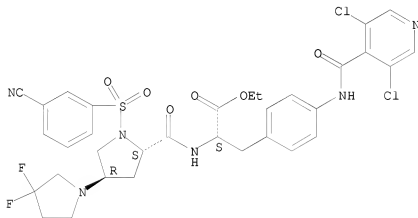
Absolute stereochemistry.



RN 877406-29-6 CAPLUS

CN L-Phenylalanine, (4R)-1-[(3-cyanophenyl)sulfonyl]-4-(3,3-difluoro-1-pyrrolidinyl)-L-prolyl-4-[[[(3,5-dichloro-4-pyridinyl)carbonyl]amino]-ethyl ester (9CI) (CA INDEX NAME)

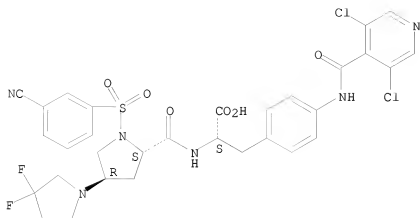
Absolute stereochemistry.



RN 877406-30-9 CAPLUS

CN L-Phenylalanine, (4R)-1-[(3-cyanophenyl)sulfonyl]-4-(3,3-difluoro-1-pyrrolidinyl)-L-prolyl-4-[[[(3,5-dichloro-4-pyridinyl)carbonyl]amino]-ethyl ester (9CI) (CA INDEX NAME)

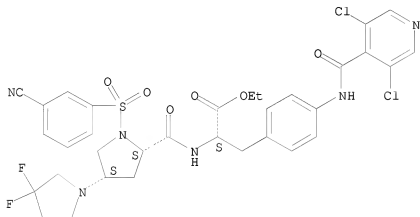
Absolute stereochemistry.



RN 877406-32-1 CAPLUS

CN L-Phenylalanine, (4S)-1-[(3-cyanophenyl)sulfonyl]-4-(3,3-difluoro-1-pyrrolidinyl)-L-prolyl-4-[[(3,5-dichloro-4-pyridinyl)carbonyl]amino]-ethyl ester (9CI) (CA INDEX NAME)

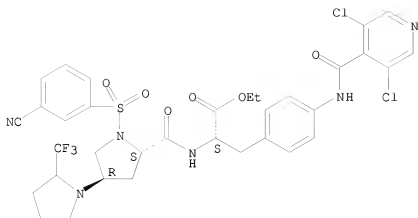
Absolute stereochemistry.



RN 877406-43-4 CAPLUS

CN L-Phenylalanine, (4R)-1-[(3-cyanophenyl)sulfonyl]-4-[2-(trifluoromethyl)-1-pyrrolidinyl]-L-prolyl-4-[[(3,5-dichloro-4-pyridinyl)carbonyl]amino]-ethyl ester (9CI) (CA INDEX NAME)

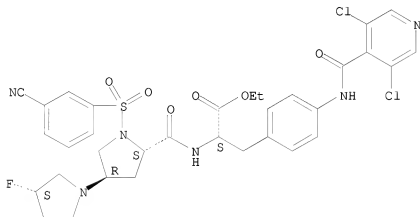
Absolute stereochemistry.



RN 877406-45-6 CAPLUS

CN L-Phenylalanine, (4R)-1-[(3-cyanophenyl)sulfonyl]-4-[(3S)-3-fluoro-1-pyrrolidinyl]-L-prolyl-4-[[3,5-dichloro-4-pyridinyl]carbonyl]amino]-ethyl ester (9CI) (CA INDEX NAME)

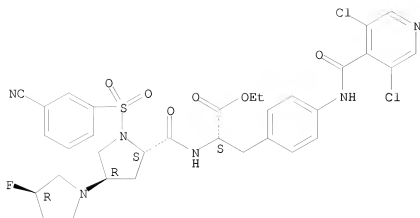
Absolute stereochemistry.



RN 877406-47-8 CAPLUS

CN L-Phenylalanine, (4R)-1-[(3-cyanophenyl)sulfonyl]-4-[(3R)-3-fluoro-1-pyrrolidinyl]-L-prolyl-4-[[3,5-dichloro-4-pyridinyl]carbonyl]amino]-ethyl ester (9CI) (CA INDEX NAME)

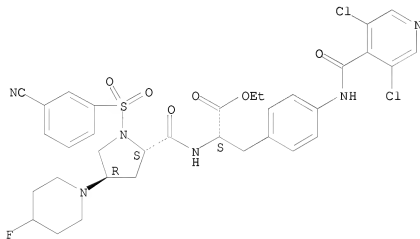
Absolute stereochemistry.



RN 877406-49-0 CAPLUS

CN L-Phenylalanine, (4R)-1-[(3-cyanophenyl)sulfonyl]-4-(4-fluoro-1-piperidinyl)-L-prolyl-4-[[[(3,5-dichloro-4-pyridinyl)carbonyl]amino]-ethyl ester (9CI) (CA INDEX NAME)

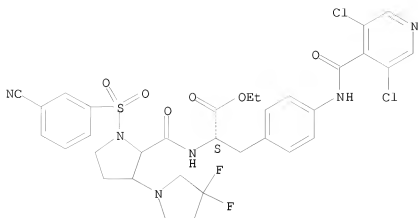
Absolute stereochemistry.



RN 877406-51-4 CAPLUS

CN L-Phenylalanine, 1-[(3-cyanophenyl)sulfonyl]-3-(3,3-difluoro-1-pyrrolidinyl)-L-prolyl-4-[[[(3,5-dichloro-4-pyridinyl)carbonyl]amino]-ethyl ester (9CI) (CA INDEX NAME)

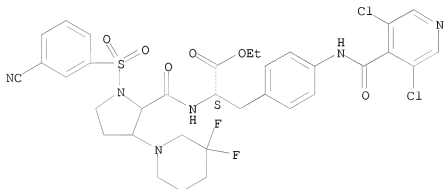
Absolute stereochemistry.



RN 877406-53-6 CAPLUS

CN L-Phenylalanine, 1-[(3-cyanophenyl)sulfonyl]-3-(3,3-difluoro-1-piperidinyl)prolyl-4-[[[(3,5-dichloro-4-pyridinyl)carbonyl]amino]-, ethyl ester (9CI) (CA INDEX NAME)

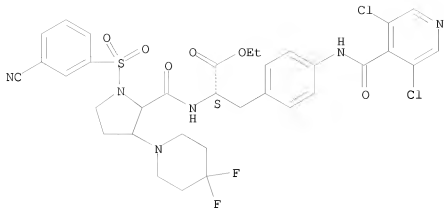
Absolute stereochemistry.



RN 877406-55-8 CAPLUS

CN L-Phenylalanine, 1-[(3-cyanophenyl)sulfonyl]-3-(4,4-difluoro-1-piperidinyl)prolyl-4-[[[(3,5-dichloro-4-pyridinyl)carbonyl]amino]-, ethyl ester (9CI) (CA INDEX NAME)

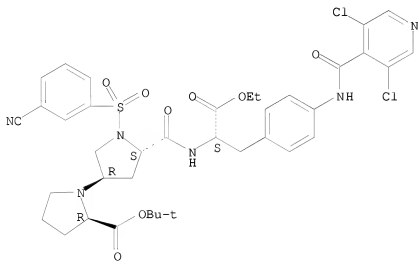
Absolute stereochemistry.



RN 877406-57-0 CAPLUS

CN L-Phenylalanine, (4R)-1-[(3-cyanophenyl)sulfonyl]-4-[(2R)-2-[(1,1-dimethylethoxy)carbonyl]-1-pyrrolidinyl]-L-prolyl-4-[[[(3,5-dichloro-4-pyridinyl)carbonyl]amino]-, ethyl ester (9CI) (CA INDEX NAME)

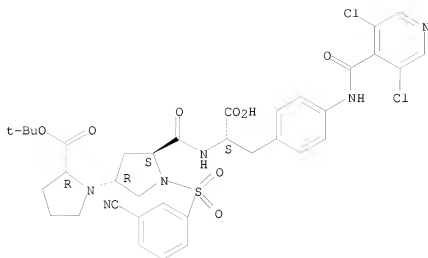
Absolute stereochemistry.



RN 877406-58-1 CAPLUS

CN L-Phenylalanine, (4R)-1-[(3-cyanophenyl)sulfonyl]-4-[(2R)-2-[(1,1-dimethylethoxy)carbonyl]-1-pyrrolidinyl]-L-prolyl-4-[[[(3,5-dichloro-4-pyridinyl)carbonyl]amino]- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



IT 877406-28-5P 877406-31-0P 877406-33-2P
 877406-34-3P 877406-35-4P 877406-36-5P
 877406-37-6P 877406-38-7P 877406-41-2P
 877406-42-3P 877406-44-5P 877406-46-7P
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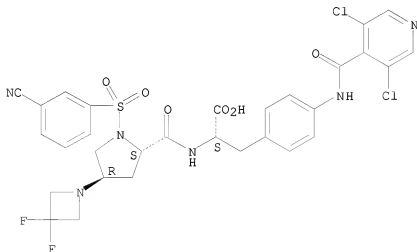
RL: PAC (Pharmacological activity); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)

(preparation of dipeptide derivs. as VLA-4 antagonists)

RN 877406-28-5 CAPLUS

CN L-Phenylalanine, (4R)-1-[(3-cyanophenyl)sulfonyl]-4-(3,3-difluoro-1-azetidiny)-L-prolyl-4-[[[(3,5-dichloro-4-pyridinyl)carbonyl]amino]- (9CI) (CA INDEX NAME)

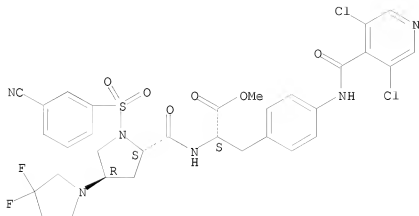
Absolute stereochemistry.



RN 877406-31-0 CAPLUS

CN L-Phenylalanine, (4R)-1-[(3-cyanophenyl)sulfonyl]-4-(3,3-difluoro-1-pyrrolidinyl)-L-prolyl-4-[[[(3,5-dichloro-4-pyridinyl)carbonyl]amino]-, methyl ester (9CI) (CA INDEX NAME)

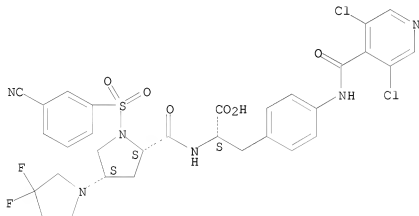
Absolute stereochemistry.



RN 877406-33-2 CAPLUS

CN L-Phenylalanine, (4S)-1-[(3-cyanophenyl)sulfonyl]-4-(3,3-difluoro-1-pyrrolidinyl)-L-prolyl-4-[[(3,5-dichloro-4-pyridinyl)carbonyl]amino]-(9CI) (CA INDEX NAME)

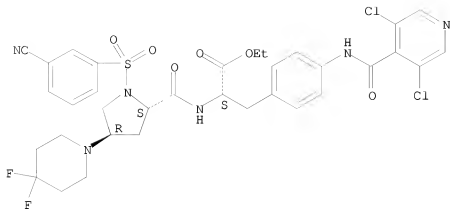
Absolute stereochemistry.



RN 877406-34-3 CAPLUS

CN L-Phenylalanine, (4R)-1-[(3-cyanophenyl)sulfonyl]-4-(4,4-difluoro-1-piperidinyl)-L-prolyl-4-[[(3,5-dichloro-4-pyridinyl)carbonyl]amino]-ethyl ester (9CI) (CA INDEX NAME)

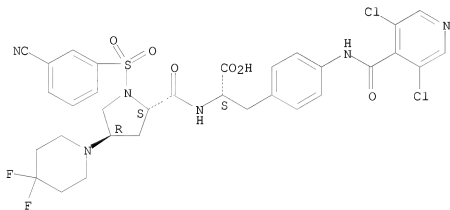
Absolute stereochemistry.



RN 877406-35-4 CAPLUS

CN L-Phenylalanine, (4R)-1-[(3-cyanophenyl)sulfonyl]-4-(4,4-difluoro-1-piperidinyl)-L-prolyl-4-[[[(3,5-dichloro-4-pyridinyl)carbonyl]amino]- (9CI)
(CA INDEX NAME)

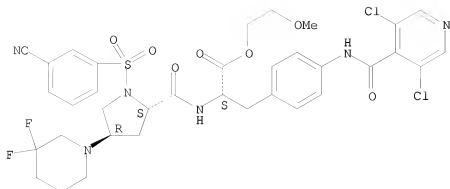
Absolute stereochemistry.



RN 877406-36-5 CAPLUS

CN L-Phenylalanine, (4R)-1-[(3-cyanophenyl)sulfonyl]-4-(3,3-difluoro-1-piperidinyl)-L-prolyl-4-[[[(3,5-dichloro-4-pyridinyl)carbonyl]amino]-, 2-methoxyethyl ester (9CI) (CA INDEX NAME)

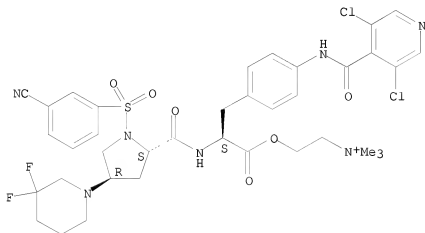
Absolute stereochemistry.



RN 877406-37-6 CAPLUS

CN L-Phenylalanine, (4R)-1-[(3-cyanophenyl)sulfonyl]-4-(3,3-difluoro-1-piperidinyl)-L-prolyl-4-[[(3,5-dichloro-4-pyridinyl)carbonylamino]-, 2-(trimethylammonio)ethyl ester (9CI) (CA INDEX NAME)

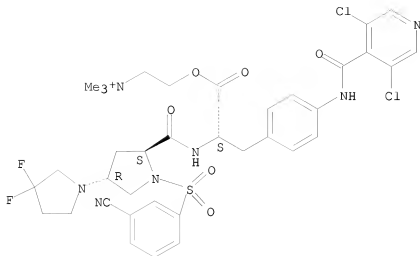
Absolute stereochemistry.



RN 877406-38-7 CAPLUS

CN L-Phenylalanine, (4R)-1-[(3-cyanophenyl)sulfonyl]-4-(3,3-difluoro-1-pyrrolidinyl)-L-prolyl-4-[[(3,5-dichloro-4-pyridinyl)carbonylamino]-, 2-(trimethylammonio)ethyl ester (9CI) (CA INDEX NAME)

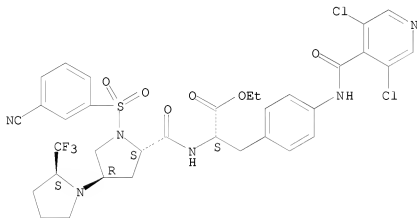
Absolute stereochemistry.



RN 877406-41-2 CAPLUS

CN L-Phenylalanine, (4R)-1-[(3-cyanophenyl)sulfonyl]-4-[(2S)-2-(trifluoromethyl)-1-pyrrolidinyl]-L-prolyl-4-[(3,5-dichloro-4-pyridinyl)carbonylamino]-, ethyl ester (9CI) (CA INDEX NAME)

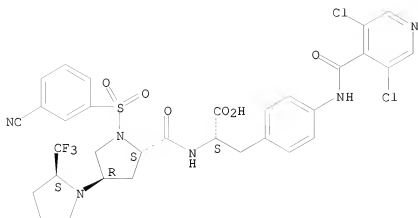
Absolute stereochemistry.



RN 877406-42-3 CAPLUS

CN L-Phenylalanine, (4R)-1-[(3-cyanophenyl)sulfonyl]-4-[(2S)-2-(trifluoromethyl)-1-pyrrolidinyl]-L-prolyl-4-[(3,5-dichloro-4-pyridinyl)carbonylamino]- (9CI) (CA INDEX NAME)

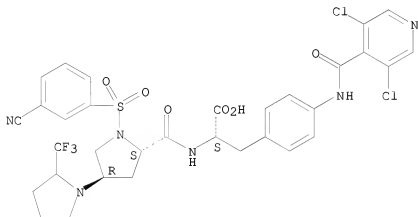
Absolute stereochemistry.



RN 877406-44-5 CAPLUS

CN L-Phenylalanine, (4R)-1-[(3-cyanophenyl)sulfonyl]-4-[2-(trifluoromethyl)-1-pyrrolidinyl]-L-prolyl-4-[[(3,5-dichloro-4-pyridinyl)carbonyl]amino]-(9CI) (CA INDEX NAME)

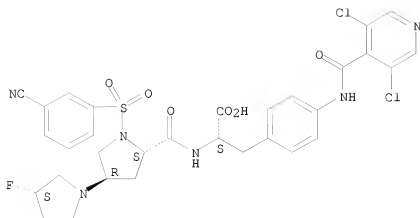
Absolute stereochemistry.



RN 877406-46-7 CAPLUS

CN L-Phenylalanine, (4R)-1-[(3-cyanophenyl)sulfonyl]-4-[(3S)-3-fluoro-1-pyrrolidinyl]-L-prolyl-4-[[(3,5-dichloro-4-pyridinyl)carbonyl]amino]-(9CI) (CA INDEX NAME)

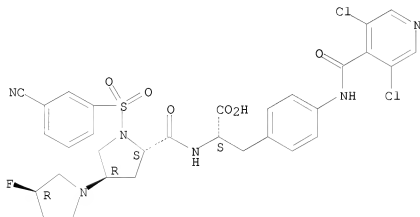
Absolute stereochemistry.



RN 877406-48-9 CAPLUS

CN L-Phenylalanine, (4R)-1-[(3-cyanophenyl)sulfonyl]-4-[(3R)-3-fluoro-1-pyrrolidinyl]-L-prolyl-4-[[(3,5-dichloro-4-pyridinyl)carbonyl]amino]-(9CI) (CA INDEX NAME)

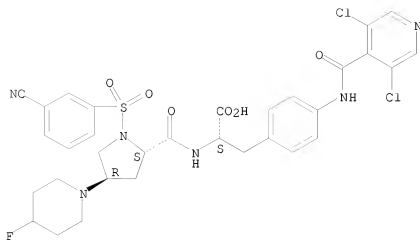
Absolute stereochemistry.



RN 877406-50-3 CAPLUS

CN L-Phenylalanine, (4R)-1-[(3-cyanophenyl)sulfonyl]-4-(4-fluoro-1-piperidinyl)-L-prolyl-4-[[(3,5-dichloro-4-pyridinyl)carbonyl]amino]-(9CI) (CA INDEX NAME)

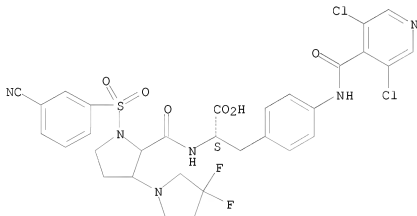
Absolute stereochemistry.



RN 877406-52-5 CAPLUS

CN L-Phenylalanine, 1-[(3-cyanophenyl)sulfonyl]-3-(3,3-difluoro-1-pyrrolidinyl)-L-prolyl-4-[[[(3,5-dichloro-4-pyridinyl)carbonyl]amino]-(9CI) (CA INDEX NAME)

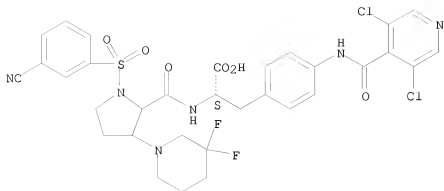
Absolute stereochemistry.



RN 877406-54-7 CAPLUS

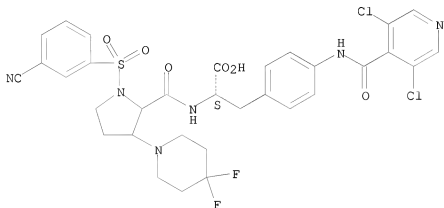
CN L-Phenylalanine, 1-[(3-cyanophenyl)sulfonyl]-3-(3,3-difluoro-1-piperidinyl)prolyl-4-[[[(3,5-dichloro-4-pyridinyl)carbonyl]amino]-(9CI) (CA INDEX NAME)

Absolute stereochemistry.



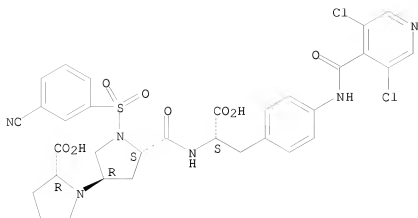
RN 877406-56-9 CAPLUS
 CN L-Phenylalanine, 1-[(3-cyanophenyl)sulfonyl]-3-(4,4-difluoro-1-piperidinyl)prolyl-4-[[[(3,5-dichloro-4-pyridinyl)carbonyl]amino]- (9CI)
 (CA INDEX NAME)

Absolute stereochemistry.



RN 877406-59-2 CAPLUS
 CN L-Phenylalanine, (4R)-4-[(2R)-2-carboxy-1-pyrrolidinyl]-1-[(3-cyanophenyl)sulfonyl]-L-prolyl-4-[[[(3,5-dichloro-4-pyridinyl)carbonyl]amino]- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



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CA SUBSCRIBER PRICE                -1.60      -2.40
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FILE 'STNGUIDE' ENTERED AT 18:41:57 ON 11 NOV 2008
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FILE CONTAINS CURRENT INFORMATION.
 LAST RELOADED: Nov 7, 2008 (20081107/UP).

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---Logging off of STN---

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Executing the logoff script...

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STN INTERNATIONAL LOGOFF AT 18:57:02 ON 11 NOV 2008